NONLINEAR METHODS FOR INVERSE PROBLEMS

A thesis
presented for the degree of
Doctor of Philosophy
in Mathematics
from the University of Canterbury,
Christchurch, New Zealand

T. John Connolly
B.Sc. (Hons), M.Sc.
August 1989

ABSTRACT

The general inverse problem is formulated as a nonlinear operator equation. The solution of this via the Newton-Kantorovich method is outlined. Fréchet differentiability of the operator is given by the implicit function theorem. We also consider questions such as uniqueness, stability and regularization of the inverse problem.

This general theory is then applied to a number of different inverse problems. The Newton-Kantorovich method is derived for each example and Fréchet differentiability examined. In some cases numerical results are provided, for others our work provides a theoretical basis for results obtained by different authors.

The problems considered include an interior measurement inverse problem from steady-state diffusion, and a boundary measurement problem for electrical conductivity imaging. We also examine the determination of refractive indices and scattering boundaries for the Helmholtz equation from measurements of the farfield. In addition an inverse problem from geometric optics is investigated.

ACKNOWLEDGEMENTS

I would like to express my sincerest thanks to Dr D.J.N. Wall, for his assistance and supervision over the years taken for this research.

I would also like to thank Dr R.J. Astley, Civil Engineering Department and Professor R.H.T. Bates, R. Murch and Dr D.G.H. Tan, all from the Electrical and Electronic Engineering Department, for useful discussions and their encouragement. In addition, I thank Mrs B. Bristowe for her typing of this thesis.

The award of a University Grants Committee postgraduate scholarship in 1984 is also gratefully acknowledged.

PREFACE

Inverse or identification problems often takes the form of determining an unknown function, which is a coefficient in a partial differential equation. Another type of inverse problem commonly encountered, in inverse scattering for example, is where the unknown quantity is a boundary of the region on which the problem is defined.

The inverse problem is distinct from the direct or forward problem, where the coefficient function or boundary of the problem is known. Then we have the partial differential equation to solve, subject to boundary conditions, if there are any.

To be able to solve the inverse problem, extra information is required in the form of measurements of the solution of the corresponding direct problem. Some inverse problems are linear in nature, often requiring the solution of an integral equation of the first kind. However, for many inverse problems, there is a nonlinear relationship between the measurements and the solution of the problem.

The approach used in this thesis to solve such inverse problems is outlined in Chapter One. We first formulate them as nonlinear operator equations by requiring the solution of the direct problem, the partial differential equation, to match the measurements. The nonlinear operator equation is then solved using the Newton-Kantorovich method. This iterative scheme linearizes the operator at each step to allow us to solve for an improved approximation. We can then utilize the highly developed theory and machinery for solving linear operator equations.

Problems such as the existence, uniqueness and characterization of solutions of the inverse problem are also outlined. In addition we consider properties of the resulting operator-such as continuity, Fréchet differentiability and compactness. The instability resulting from the compactness of the operator requires the use of regularization methods. The examination of such questions is necessary before a numerical implementation of our methods is attempted.

In Chapter Two the properties of the direct problem for the steady-state diffusion equation are examined. Existence, uniqueness and regularity results are given for both classical and weak solutions of the equation.

In Chapter Three an inverse problem from steady-state diffusion, with interior measurements, is investigated. Direct identification and the stability of the inverse problem are first reviewed. Newton methods are then derived for the solution of this inverse problem. Fréchet differentiability and compactness are shown for the nonlinear operator utilized and the application of regularization techniques outlined. In the chapter numerical results from the solution of a one-dimensional problem are given - these incorporate regularization methods in the presence of measurement noise.

In Chapter Four inverse problems for boundary scattering are considered. We utilize the implicit function theorem to obtain the continuous dependence of the farfield upon the boundary. Expressions for the Fréchet derivative of this map are derived via the null field method and also variational methods. Finally we investigate the determination of an unknown impedance boundary condition from farfield measurements and a Fréchet differentiability result is proven for this problem.

Chapter Five is concerned with the direct problem for a modified form of the Helmholtz equation - with spatially varying refractive index. Regularity results for this equation are obtained both in spaces of continuously differentiable functions and Sobolev spaces. Neumann series solutions of the equivalent integral equation formulation are also considered. Numerical solutions of the equation are discussed.

In Chapter Six we consider the determination of a spatially varying refractive index in the Helmholtz equation. This inverse problem is formulated as a non linear operator equation and the Newton-Kantorovich method for its solution derived. Fréchet differentiability is proven for both continuous refractive indices and square integrable indices for which the Born series converges. The Fréchet derivative is shown to be compact with point measurements and regularization methods examined.

Chapter Seven investigates an inverse problem from geometric optics. Newton's method and regularization techniques are outlined for the inverse problem and these are related to work of other authors.

In Chapter Eight a summary and conclusions are presented, and also some suggestions for future research relating to the work in this thesis.

During the course of my studies the following papers and report were prepared :

1. T.J. Connolly, D.J.N. Wall and R.H.T. Bates. *Inverse Problems and the Newton–Kantorovich Method.* In A.J. Devaney and R.H.T. Bates, editors, "Inverse Optics II", pages 30-34, Proceedings SPIE volume 558, August 1985.
2. T.J. Connolly and D.J.N. Wall. *An Inverse Problem, with Boundary Measurements for the Steady State Diffusion Equation,* Research Report 40, Department of Mathematics, University of Canterbury, Christchurch, New Zealand, October 1987.
3. T.J. Connolly and D.J.N. Wall. *On an Inverse Problem, with Boundary Measurements for the Steady State Diffusion Equation,* "Inverse Problems", 4 : 995-1012, 1988.

4. T.J. Connolly and D.J.N. Wall. *On Frechet Differentiability of Non–Linear Operators occurring in Inverse Problems – an Implicit Function Theorem Approach*, to be submitted to "Inverse Problems".

The third paper forms the appendix of this thesis.

Sections of the first three chapters are based upon the author's 1985 M.Sc. thesis, *Inverse Problems for an Elliptic Equation*, University of Canterbury, Christchurch, New Zealand.

NOTATION

$\mathbb{R}^N$	product of n copies of the real line $\mathbb{R}$
$\mathbb{R}_n$	dual of $\mathbb{R}^n$
$\lvert \underset{-}{x} \rvert$	$= (x_1^2 + \ldots + x_n^2)^{\frac{1}{2}}$, the euclidean norm on $\mathbb{R}^n$
sup	supremum, or least upper bound, of a set of real numbers
inf	infimum, or greatest lower bound, of a set of real numbers
Ω	bounded domain in $\mathbb{R}^n$
$\overline{\Omega}$	closure of Ω
$\partial\Omega$	$= \overline{\Omega}\backslash\Omega$, boundary of Ω
supp u	the support of u (smallest closed set outside which u = 0)
	Multi-index Notation -
Z_+^n	product of n copies of the set Z_+ of non-negative integers
$\lvert \underset{-}{\alpha} \rvert$	$= \alpha_1 + \ldots + \alpha_n$, where the n-tuple $\underset{-}{\alpha} \in Z_+^n$
$D^{\underset{-}{\alpha}}$	$= (\partial/\partial x^1)^{\alpha_1} \ldots (\partial/\partial x^n)^{\alpha_n}$, $(\underset{-}{\alpha} \in Z_+^n)$

Main Function Spaces

$C^0(\overline{\Omega})$	space of real continuous functions on the closure $\overline{\Omega}$ (supposed to be compact) of Ω, equipped with the maximum norm
$C^m(\Omega)$	space of real functions, defined and m times continuously differentiable in Ω ($m \in Z_+$ or $m = +\infty$)
$B^m(\Omega)$	subspace of $C^m(\Omega)$ consisting of the functions having all their derivatives bounded in the whole of Ω

$C^m(\overline{\Omega})$ subspace of $B^m(\Omega)$ consisting of the functions all of whose derivatives of order $\leq$ m can be extended as continuous functions to the closure $\overline{\Omega}$ of Ω , equipped with the norm

$$||u|| = \max_{0 \leq |\alpha| \leq m} \sup_{\underline{x} \in \Omega} |D^\alpha u(\underline{x})|$$

$C_c^\infty(\Omega)$ subspace of $C^\infty(\Omega)$ consisting of the functions having compact support; elements of $C_c^\infty(\Omega)$ are often referred to as test functions in Ω.

$C^{m,\lambda}(\overline{\Omega})$ subspace of $C^m(\overline{\Omega})$ consisting of those functions u for which, for $0 \leq |\alpha| < m$, $D^\alpha u$ satisfies a Hölder condition of exponent λ, equipped with the norm

$$||u||_{m,\lambda} = \max_{0 \leq |\alpha| \leq m} \sup_{\substack{\underline{x}, \underline{y} \in \Omega \\ \underline{x} \neq \underline{y}}} \frac{|D^\alpha u(\underline{x}) - D^\alpha u(\underline{y})|}{|\underline{x} - \underline{y}|}$$

$L^p(\Omega)$ Lebesgue space of measurable functions u such that the pth power of the absolute value $|u|$ is integrable over Ω $(1 \leq p < +\infty)$, equipped with the norm

$$||u||_p = \left[\int_\Omega |u(x)|^p dx\right]^{1/p}$$

$L^\infty(\Omega)$ Lebesgue space of measurable functions u in Ω which are essentially bounded, equipped with the norm $||u||_\infty$, the essential supremum of $|u|$

$W^{m,p}(\Omega)$	Sobolev space of functions u in Ω such that $D^{\underline{\alpha}}u \in L^p(\Omega)$ for all n-tuples $\underline{\alpha} \in Z_+$, $\|\alpha\| \leq m$ ($D^{\underline{\alpha}}$ denotes distribution derivative)
$H^m(\Omega)$	$\equiv W^{m,2}(\Omega)$, a Hilbert space
$H^m_0(\Omega)$	closure in $H^m(\Omega)$ of $C^\infty_c(\Omega)$
$H^{-m}(\Omega)$	space of distributions u in Ω which can be written as finite sums of derivatives of order $\leq$m of functions belonging to $L^2(\Omega)$ ($m \in Z_+$)
$H^s(\mathbb{R}^n)$	the Sobolev space of order $s \in \mathbb{R}$ in $\mathbb{R}^n$, i.e. the space of tempered distributions u in $\mathbb{R}^n$ whose Fourier transform $\hat{u}$ is a measurable function such that $$\|u\|_s = \left[\int_{\mathbb{R}_n} \|\hat{u}(\xi)\|^2 (1 + \|\xi\|^2)^s \frac{d\xi}{(2\pi)^n} \right]^{\frac{1}{2}} < +\infty$$
$H^s(K)$	subspace of H^s consisting of all elements having their support contained in the compact set K

CONTENTS

CHAPTER ONE

THE GENERAL INVERSE PROBLEM

1.1 INTRODUCTION

A problem of much interest in physics and engineering is the determination of the interior properties of an object. To enable this, the object is probed with some incident field (for example electromagnetic or acoustic waves). Measurements of the resulting field are then performed either on the object's surface or exterior to it. From these measurements the relevant interior properties are to be deduced. Often the location and shape of such an object must also be determined from farfield measurements. Problems of this form arise in geophysical prospecting, nondestructive testing, remote sensing, medical imaging and related areas.

A mathematical description of the problem is the determination of a spatially-varying coefficient function in a region. This function is generally a coefficient in a partial differential equation. Knowledge of the solution of this equation is used to determine the coefficient function.

The conventional solution of the partial differential equation (p.d.e.) is known as the direct problem. That of determining the coefficient function is known as the inverse or identification problem. A selection of review papers on inverse problems is Boerner *et al.* [1981], Parker [1977a], Polis and Goodson [1976], Sabatier [1983] and Sleeman [1982].

In this thesis we formulate the inverse problem as a nonlinear operator equation. The use of iterative methods is investigated to solve such an equation. A certain amount of functional analysis in a Banach space setting is utilized in order to examine the properties of the operator equation. In this chapter we first consider a general class of inverse problem. The methods outlined are then applied to solving particular problems in later chapters.

1.2 THE GENERAL PROBLEM

We denote by $v(\underline{x})$ the spatially varying function to be determined on a region Ω, such as in Figure 1.1. This function is a coefficient in a partial differential equation (or perhaps an integral equation). The solution of this equation is denoted by $y(\underline{x})$.

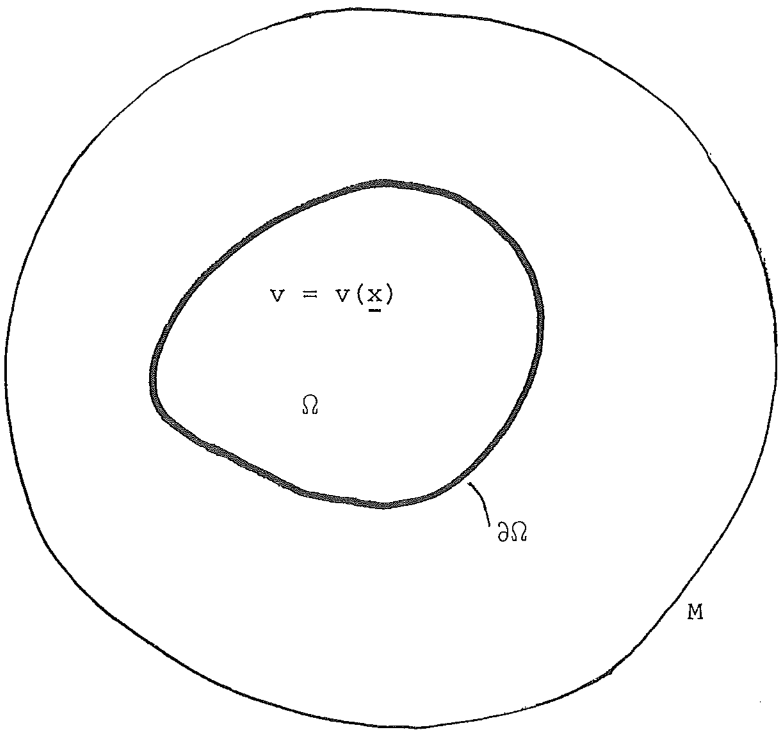

Figure 1.1

The problem will be considered in a function space setting. The coefficient function, v, is required to belong to a subset, X_0, of a Banach space X. The direct problem solution, y, is also in some Banach space, Y. For example, if the direct problem is a nth order partial differential equation then Y is a space of n times continuously differentiable functions (typically $C^n(\overline{\Omega})$).

We shall assume the functions v and y are related by an operator equation of the form

$$\xi(v,y) = 0 \ . \tag{1.1}$$

Here $\xi : X_0 \otimes Y \to W$, where W is another Banach space. This equation incorporates possible initial/boundary conditions on y - ξ then maps into a product space resulting from the differential equation and the additional conditions.

The partial differential equation in question is generally defined on either of two types of regions. Firstly, it is defined on a compact region such as Ω in Figure 1.1, then the measurements of the direct problem solution are made on the boundary $\partial\Omega$. Alternatively, the equation may be defined on an unbounded region containing Ω - such as $\mathbb{R}^n$. This situation occurs often in wave propagation problems. Then measurements are made on a surface, M, exterior to Ω and the coefficient function, v, is known outside Ω.

We do however consider one problem where the measurements may be performed in the interior of Ω. Such problems though are generally easier to solve than the corresponding boundary or exterior measurement problems.

Inverse problems resulting from several different direct problems shall be tackled in this thesis.

(i) An example that will be considered in much more detail in later chapters is the following elliptic p.d.e. (with Dirichlet boundary conditions), occurring in steady-state heat and electric current flow :

$$\begin{aligned} \nabla\cdot(f(\underline{x})\nabla\phi(\underline{x})) &= 0\,, \quad \underline{x} \in \Omega \\ \phi(\underline{x}) - g(\underline{x}) &= 0, \quad \underline{x} \in \partial\Omega \ . \end{aligned} \tag{1.2}$$

Here the function to be reconstructed, f, corresponds to v in (1.1), and the solution of the direct problem ϕ corresponds to y. An alternative boundary condition for this problem is the Neumann condition

$$f(\underset{\sim}{x}) \frac{\partial \phi(\underset{\sim}{x})}{\partial n} - h(\underset{\sim}{x}) = 0 , \quad \underset{\sim}{x} \in \partial \Omega .$$

Here $\frac{\partial}{\partial n}$ denotes the normal derivative to the boundary.

(ii) Another problem considered in this thesis is for the modified Helmholtz equation

$$\Delta \psi(\underset{\sim}{x}) + k^2 n^2(\underset{\sim}{x}) \psi(\underset{\sim}{x}) = 0 , \quad \underset{\sim}{x} \in \mathbb{R}^n ,$$

where ψ is the field and a spatially-varying refractive index, n, is to be reconstructed. Closely related to this is the Schrödinger equation

$$\Delta \psi(\underset{\sim}{x}) + k^2 \psi(\underset{\sim}{x}) = V(\underset{\sim}{x}) \psi(\underset{\sim}{x}) , \quad \underset{\sim}{x} \in \mathbb{R}^n ,$$

where ψ is the probability density function and V the potential. Both these equations arise in wave propagation problems and are subject to a condition at infinity known as the radiation condition. The determination of a scattering boundary in the Helmholtz equation proper (i.e. with n = 1) is also examined.

We may consider that examining these elliptic partial differential equations as examples is not much of a restriction. This is because such equations are obtained from the Fourier/Laplace transformation of corresponding hyperbolic or parabolic time domain equations. Also, our methods may easily be applied to problems in the time domain itself. In addition we discuss the extensions from the above scalar equations to the corresponding vector-valued problems.

1.2.1 *An Operator Equation*

The measurements can in general be explicitly dependent upon the function v, in addition to the direct problem solution, y. This quantity to be measured is denoted by B(v,y). Σ shall denote the measurements that are made of B(v,y). Σ is required to be in some Banach space, Z.

If v^* is the actual coefficient function then

$$\Sigma = B(v^*,y(v^*)) + \epsilon \ ,$$

where $y(v^*)$ is the direct problem solution resulting from the coefficient v^*. The function $\epsilon(\underline{x})$, $\underline{x} \in M$ is the noise incurred during measurement. M is the region where the measurements are performed - see Figure 1.1. We note that M is $\partial\Omega$ in many problems (these are often called boundary measurement problems).

The inverse problem may then be formulated as the operator equation

$$P(v) = B(v,y(v)) - \Sigma = 0 \ , \qquad \underline{x} \in M \ , \tag{1.3}$$

with $P: X_0 \rightarrow Z$. The function y(v) is the solution of the direct problem given by $\xi(v,y(v)) = 0$.

There is in general a nonlinear relationship between the measurements and the function to be reconstructed. $P(v) = 0$ is then a nonlinear operator equation. To solve this equation we shall consider in depth in this thesis the use of the Newton-Kantorovich iterative method.

In the example from steady-state diffusion (1.2) with a Dirichlet condition, consider measurements made of the normal current, $f \dfrac{\partial\phi}{\partial n}$, on the boundary -

denote these by $\tilde{\Phi}$. The operator equation to be solved would then be as follows

$$T(f) = f(\underset{-}{x}) \frac{\partial \phi}{\partial n}(f,\underset{-}{x}) - \tilde{\Phi}(\underset{-}{x}) = 0 , \quad \underset{-}{x} \in \partial\Omega . \tag{1.4}$$

Here $\phi(f)$ is the direct problem solution with coefficient f.

Another problem of much interest is the inverse boundary scattering problem for wave propagation problems. Here instead of determining an unknown coefficient function, the location and shape of the boundary, $\partial\Omega$ of the scattering obstacle are to be determined. This inverse problem may also be formulated as a nonlinear operator equation and iterative schemes such as the Newton-Kantorovich method used to solve it (Colton [1984], Wall *et al.* [1985] and Murch, Tan and Wall [1988]). We consider this problem in more detail in Chapter 8.

1.2.2 *Existence and Characterization*

Denote by v^* the function to be reconstructed - that from which the measurements arise. Then in the absence of measurement noise the measurement function $\Sigma = B(v^*,y(v^*))$. Clearly there then exists a solution to the inverse problem, v^* as

$$P(v^*) = 0 .$$

However, if measurement noise is present it is possible there does not exist a function v such that

$$\Sigma = B(v,y(v)) .$$

Then a solution to the operator equation does not exist in the classical sense.

An important question is then the characterization problem. That is given an arbitrary measurement function Σ, can we determine whether or not it may have arisen from some function v. That is we require necessary and sufficiency conditions on $\Sigma = B(v,y(v))$ to hold for some $v \in X_0$. Equivalently the range of the operator B, R(B), is to be determined as a subset of the measurement space Z.

Clearly Σ will have to require certain smoothness assumptions consistent with being obtained from a solution of the differential equation, but going beyond this is generally difficult. However, the characterization problem has been examined for particular inverse scattering problems in Colton and Kress [1983], Colton [1984], Ramm [1987a,b], and Newton [1982].

Such problems as existence of solutions arise as generally P(v) is a compact operator and so functions in the range of B, $\mathbb{R}$(B), are smoother than those in the measurement space, denoted by Z. We note questions of existence of solutions to such equations are closely related to those of stability.

In §1.3 we consider the application of regularization techniques - where the inverse problem is reformulated so that the existence and continuous dependence upon measurement data of solutions is obtained.

1.2.3 *Uniqueness*

Knowledge of uniqueness of a solution to the equation P(v) = 0 provides a minimum measurement set for practical methods of solving the inverse problem. However, this is often fairly difficult to establish - there exist no general results and each inverse problem must be treated individually. For many problems, including the ones considered later, much work needs to be done. We shall briefly preview here the different techniques used for the problems of this thesis.

Firstly, the interior measurement problem considered in Chapter Three - which has an elliptic p.d.e. for the direct problem - may be formulated as a hyperbolic p.d.e. for the inverse problem. In addition to providing uniqueness results, this may be solved directly in some circumstances.

For the boundary measurement version of this problem (which we consider in Chapter Three and the Appendix) Kohn and Vogelius [1984] use highly oscillatory boundary data to show the conductivity and all its derivatives are uniquely determined on the boundary. It then follows by analytic continuation that a real analytic conductivity may be uniquely determined by boundary measurements.

Much of the difficulty in proving uniqueness results for inverse problems is due to their nonlinearity. On the other hand linearized inverse problems can often be expressed as integral equations of the first kind with the kernel being determined analytically. Then the uniqueness or otherwise for the problem is much easier to establish. In particular, Calderon [1980] has proven uniqueness for the conductivity determination inverse problem - linearized about a constant. In the Appendix we give another such result for this problem, using the completeness of the solutions of the p.d.e. which determine the kernel. Also there are uniqueness results available with the Born approximation, which we show in Chapter Six to be the linearization of the inverse problem of determining a refractive index in the Helmholtz equation.

For several nonlinear one-dimensional inverse problems there are uniqueness results - these are based upon the use of spectral theory and the work of Gelfand and Levitan [1956]. In particular results for the problem of determining a radially symmetric refractive index in the Helmholtz equation (or potential in the Schrödinger equation) are to be found in Chadan and Sabatier [1977]. Kohn and Vogelius [1985] also prove such a result for a one-dimensional form of the electrical conductivity determination problem.

A three-dimensional refractive index in the Helmholtz equation is also uniquely determined by knowledge of the far field pattern at a single frequency. This result due to Ramm [1987] is based upon the completeness of products of solutions of the partial differential equation.

In addition it is known (Colton and Sleeman [1983] and Jones [1985] - see also Lax and Phillips [1967]) that a scattering boundary in the Helmholtz equation is uniquely determined by knowledge of the far field resulting from a finite number of incident waves at a single frequency. The proof is nonconstructive and uses the properties of the eigenvalues/eigenfunctions of the Laplacian. This particular inverse problem is considered in more detail in Chapter Four.

It is apparent from the diversity of approaches we have just outlined, that a general theory for the uniqueness of inverse problems is unlikely. However, this is not the case for the important questions of the stability and construction of solutions. We provide generally applicable approaches to these two problems in the following sections.

1.3 STABILITY

1.3.1 *Ill–posed Problems*

We shall find that for the majority of our problems the operator P(v) is compact. Compact operators are smoothing operators and do not have bounded inverses. So we cannot expect the solution of the inverse problem to depend upon the measurements in a continuous manner. Small changes in the measurement function may cause arbitrarily large changes in the solution of the operator equation (if it exists). Numerically this manifests itself as highly oscillatory and hence physically unrealistic solutions. Such inverse problems are examples of ill-posed problems.

The classic example of a linear ill-posed problem is the Fredholm integral equation of the first kind for f(x) given data g(x)

$$\int_a^b k(x,x')\, f(x')dx' = g(x) \ , \ c \leq x \leq d \, . \tag{1.5}$$

Assume the kernel k is continuous and take the function $f_n(x) = \sin(nx)$. Then from the well-known Riemann-Lebesgue theorem

$$\lim_{n\to\infty} \int_a^b k(x,x')\, f_n(x')dx' = 0 \ .$$

It follows that widely differing functions f give approximately the same data g.

We can restore the continuous dependence of the solution of the inverse problem upon the measurement functions with the use of regularization techniques. These impose constraints on the solution in order to obtain physically realistic solutions.

For most of our problems the Fréchet derivative of P(v) is a compact linear operator and in fact an integral equation of the first kind. Now the singular values of a compact linear operator, which we denote by $\{u_i\}$ are either finite (when the kernel is degenerate) or countably infinite with $u_i \to 0$ as $i \to \infty$ (see Wouk [1979] p.227). The degree of ill-conditioning of the problem depends upon the rate of decay of these singular values. If the singular values decay to zero slowly, the inverse problem may be classified as mildly ill-posed. If the decay rate is rapid - exponential decay for instance - then the problem is severely ill-posed. Also it should be noted that the rate of decay influences the nature of the continuous dependence obtained using regularization techniques. The faster the rate of decay, the weaker is the continuity that results. The reader is referred to Betero *et al.* [1979] for a more detailed discussion of all these questions as they apply to linear inverse problems.

1.3.2 *Regularization Methods*

The numerical instabilities and ill-posed nature of this problem suggest a regularization approach. "Regularization" of a problem refers in general to solving a related problem, called the regularized problem, the solution of which is more regular, in a sense, than that of the original problem and approximates the solution of the original problem. When referring to ill-posed problems, regularization is an approach to circumvent lack of continuous dependence on the data. The regularized problem is a well-posed problem (i.e. has a bounded inverse) whose solution yields a physically meaningful answer to the ill-posed problem.

For an overview of regularization methods see Tikhonov and Arsenin [1977] or Nashed [1981] and for their application to inverse problems Betero *et al.* [1979].

Assume the nonlinear operator P(v) maps X $\rightarrow$ Z, where X and Z are Banach spaces. Moreover, we require P to be a continuous operator. Methods for showing the continuity of P based upon the implicit function theorem are outlined in §1.5.

Perhaps the simplest example of a regularization scheme is the Tikhonov selection method. Instead of solving the operator equation

$$P(v) = B(v,y(v)) - \Sigma = 0$$

the inverse problem is reformulated as

$$\min_{v \in X_0} ||P(v)||_Z = \min_{v \in X_0} ||B(v,y(v)) - \Sigma||_Z \ . \tag{1.6}$$

Here X_0 is chosen to be a compact subset of the space X. This generally involves constraints upon the derivatives of v.

As the problem (1.6) involves the minimization of a continuous functional over a compact set, the existence of a solution is guaranteed - see §1.5 for a proof of this result. In addition, the requirement $v \in X_0$ will give physically realistic solutions.

There is also a continuous dependence result for such solutions upon the measurement data in Colton and Kress [1983] p.238. This states if there is a sequence of functions converging to the measurement function Σ, then the resulting sequence of solutions of the minimization problem (1.6) contains a convergent subsequence. Every limit point is a solution of the minimization problem with measurement function Σ. There need not be a unique solution to the minimization problem for this result to apply.

A more sophisticated approach is to use what is known as Miller-Tikhonov regularization. Here the measurement space Z is a Hilbert space - typically L^2. The solution is required to belong to a more regular space R, where R is a Hilbert space and the imbedding operator from R into X is compact.

In this approach the constraint is combined in the functional to be minimized. That is, we wish to solve

$$\min_{v \in R} \left\{ ||P(v)||_Z^2 + \beta ||v||_R^2 \right\} \tag{1.7}$$

where $\beta > 0$ is the regularization parameter.

Continuous dependence results for such a scheme have been proven by several authors. They take the following form. Assume v^* is the true value of the coefficient v. Provided that β is an appropriately chosen function of the measurement error, any minimizer of the above functional (1.7) converges (in the norm of X) to v^*, as the measurement error tends (in the norm of Z) to zero. Results of this nature have been proven for the first kind integral equations by Tikhonov and Arsenin [1977], linear inverse problems by Betero *et.al.* [1979] and for nonlinear inverse problems by Kravaris and Seinfeld [1984]. The result in this last paper requires a unique solution to the inverse problem.

Betero *et al.* found for their problems the nature of the continuity obtained (be it logarithmic, Hölder or whatever) is dependent upon the rate of decay to zero of the singular values of the appropriate compact linear operator. This is to be expected as the degree of ill-conditioning of the problem is also dependent upon the rate of decay of these singular values.

We discuss regularization methods based upon singular value decomposition techniques, available for the solution of liner compact operator equations, in §3.4. There we also apply them to the numerical solution of a linear inverse problem in the presence of measurement noise and obtain very satisfactory results.

Another popular regularization method for linear inverse problems is the Backus-Gilbert method (from Backus and Gilbert [1970]). This technique also relies upon restricting the solution to a compact set - see Colton and Kress [1983], Chapter Seven.

We briefly mention an alternative regularization method, the linear functional strategy (see Anderssen [1980] or Elden [1988] for example). Here an appropriate functional on the solution is computed rather than the solution itself. The problem of computing such a functional can be considerably less ill-posed than the original problem.

1.4 CONSTRUCTION OF SOLUTIONS

In some special cases there exist direct (non-iterative) methods of solution for nonlinear inverse problems. In particular, methods based upon the work of Gelfand and Levitan [1955] have been used to solve inverse scattering problems. However, these methods are only applicable to specific problems and are not always practical for computational purpose. For nonlinear inverse problems generally, either an approximate or iterative method must be used to construct solutions.

1.4.1 *Linearized Problem*

A common approximate method of solution is to linearize the inverse problem about a given coefficient function, v_0. This then gives a linear operator equation to solve for an approximate solution to the nonlinear inverse problem.

Formally using the Fréchet derivative $P'(v)$ of the nonlinear operator, the linear operator equation to be solved for the approximate solution v is

$$P'(v_0)(v - v_0) = - P(v_0) \quad . \tag{1.8}$$

See §1.5.2 for a formal definition of the Fréchet derivative.

This method is valid when the function to be reconstructed v^* lies close to the given function v_0, that is

$$||v^* - v_0|| << 1$$

using an appropriate norm. As is shown in Chapter Six, the well-known Born approximation used to solve inverse scattering problems is an example of such a method.

Usually the function v_0 is fairly simple - often just a constant. This generally allows the Fréchet derivative to be determined analytically. In some cases it may also be inverted analytically giving an explicit solution to the linearized inverse problem.

We note the question of uniqueness of solutions to the linearized equation (1.8) in general can be dealt with much easier than for the nonlinear equation $P(v) = 0$.

Generally the linearized inverse problem (1.8) may be rewritten as the following integral equation of the first kind to be solved for v

$$\int_{\Omega} k(\underline{x},\underline{x}') \, v(\underline{x}') \, d\underline{x}' = \tilde{\Sigma}(\underline{x}) \, , \, \underline{x} \in M \, . \tag{1.9}$$

Here $k(\underline{x},\underline{x}')$ is a known kernel function (from the Fréchet derivative) and the right hand side $\tilde{\Sigma}$ is related to the measurement function Σ. We note that for our problems $k(\underline{x},\underline{x}')$ must often be computed numerically.

If an analytic inversion is not available, then to solve the integral equation the collocation method may be used (Baker [1977]). The unknown function is expressed as a sum of N_1 basis functions

$$v(\underline{x}) = \sum_{j=1}^{N_1} a_j g_j(\underline{x}) \; .$$

The integral equation (1.9) is then evaluated at a set of N_2 points $\{x_i\}$ - this requires measurements to be available at these points. This gives a system of equations to be solved for $\underline{a}$

$$\sum_{j=1}^{N} A_{ij} \, a_j = \tilde{\Sigma}(\underline{x}_i) \, , \, i \in \{1, ..., N_2\}$$

where

$$A_{ij} = \int_{\Omega} k(\underline{x}_i,\underline{x}') \, g_j(\underline{x}') \, d\underline{x}' \; .$$

Generally $N_2 \geq N_1$ and the system may be overdetermined and so must be solved in the least squares sense. More general methods of solution for the integral equation - utilizing test functions - such as the Petrov-Galerkin method (see Milne [1980] p.367 for example) may be utilized.

Due to the ill-posed nature of the inverse problem generally, the system of equations will be ill-conditioned. Then in the presence of measurement noise (i.e. noise in $\tilde{\Sigma}$) regularization techniques must be incorporated into solving the problem.

1.4.2 *The Fréchet Derivative*

The use of (1.8) as an approximate method of solving inverse problems was suggested in Sabatier [1972]. This author considered problems in the class given by

$$D_0(\underset{\sim}{x})y = vy$$

where $D_0(\underset{\sim}{x})$ is a "well-known" (partial differential) operator in $\mathbb{R}^n$. An expression for the Fréchet derivative of the map $v \rightarrow y(v)$ is given for v in the space of integrable functions. This is obtained by reformulating the differential equation as an integral equation using a Green's function (when this is possible) and then utilizing Newmann series and perturbation methods. The well-known Born approximation from scattering theory is given as an example of such a Fréchet derivative.

In what follows we show how to derive the Fréchet derivative for the appropriate map arising from the much wider class of problems given by (1.1), that is

$$\xi(v,y) = 0 \ .$$

The expression for the Fréchet derivative may be formalized in general function spaces using the implicit function theorem. We also show how the Fréchet derivative may be used in the Newton-Kantorovich method to reconstruct arbitrary coefficient functions, v.

So to implement either the linearization method given by (1.8) or the Newton-Kantorovich iterative scheme which is outlined later, we need to be able to compute the Fréchet derivative for the nonlinear operator P(v).

From the nonlinear operator equation (1.3) and the chain rule

$$P'(v)s = B_v(v,y(v))s + B_y(v,y(v))\, y'(v)s. \tag{1.10}$$

B_v and B_y denote partial Fréchet derivatives with respect to v and y. The function s belongs to the Banach space X.

For example, in the steady-state diffusion/electric current flow problem outlined earlier, where the normal current is measured, we have the operator

$$T(f) = f\frac{\partial}{\partial n}\phi(f) - \tilde{\Phi} \ , \quad \underset{\sim}{x} \in \partial\Omega \ .$$

$\tilde{\Phi}$ denotes the measurements of the normal current on the boundary.
It then follows that as in (1.12)

$$T'(f)s = s\frac{\partial\phi(f)}{\partial n} + f\frac{\partial}{\partial n}\phi'(f)s \ , \qquad \underset{\sim}{x} \in \partial\Omega \ .$$

The Fréchet derivative $y'(v)$ (or $\phi'(f)$ in our example) is computed from the direct problem formulation (see §1.2)

$$\xi(v,y) = 0 \ .$$

Differentiating this with respect to v gives

$$\xi_v(v,y(v))s + \xi_y(v,y(v))\, y'(v)s = 0 \ .$$

Hence

$$y'(v)s = - [\xi_y(v,y(v)]^{-1}\, \xi_v(v,y(v))s \tag{1.11}$$

assuming ξ_y^{-1} exists. This result is made rigorous in §1.5 using the implicit function theorem.

In our example (1.2)

$$\nabla\cdot[f\nabla\phi(f)] = 0 \ , \ \underset{\sim}{x} \in \Omega$$
$$\phi(f) = g \ , \ \underset{\sim}{x} \in \partial\Omega \ .$$

Differentiating with respect to f gives

$$\nabla\cdot[s\nabla\phi(f)] + \nabla\cdot[f\nabla\phi'(f)s] = 0 \ , \underset{\sim}{x} \in \Omega$$
$$\phi'(f)s = 0 \ , \underset{\sim}{x} \in \Omega \ .$$

It follows that

$$\phi'(f)s = - \int_\Omega G(f;\underset{\sim}{x},\underset{\sim}{x}')\, \nabla'\cdot[s(\underset{\sim}{x}')\, \nabla'\phi(f;\underset{\sim}{x}')]dV' \ ,$$

where $G(f;\underset{\sim}{x},\underset{\sim}{x}')$ is the Green function for (1.2) (which is dependent upon f). The solution of inverse problems for (1.2) using the Newton-Kantovovich method is considered in much more detail in Chapter Three.

We see that the Fréchet derivative, $\phi'(f)$, is an integral operator with a Green function forming part of the kernel. This is fairly typical of the problems considered in this thesis, although not always the case.

1.4.3 *Newton–Kantorovich Method*

In many practical situations the linearization method just outlined will not be applicable - often an approximation, v_0, to the solution is not known. Then we must resort to an iterative technique to solve the nonlinear operator equation.

One iterative scheme that may be used for the solution of inverse problems is the Newton-Kantorovich method (see Rall [1969]). This scheme linearizes the nonlinear operator equation about the current approximation, giving a linear operator equation to solve for the update at each iteration. This is essentially an iterative extension of the approximate method (1.8).

The Newton-Kantorovich method is then the following iterative scheme

$$v^{(k+1)} = v^{(k)} + v^{(k)} \quad , \ k = 0, 1, 2, \ldots$$

where the update $s^{(k)}$ satisfies the linear operator equation

$$P'(v^{(k)})\, s^{(k)} = -\, P(v^{(k)}) \quad . \tag{1.12}$$

The modified form of the Newton-Kantorovich method may also be used. For this method the Fréchet derivative is left fixed as at the first iteration. Then $s^{(k)}$ satisfies

$$P'(v^{(0)})\, s^{(k)} = -\, P(v^{(k)}) \quad . \tag{1.13}$$

A constant initial approximation may be used, then the comments about the analytic determination and inversion of the Fréchet derivative in the previous subsection apply.

With the modified Newton-Kantorovich method, often a consideration part of the computational work at each iteration is eliminated. However, as is to be expected, the rate of convergence suffers. If $P(v)$, $[P'(v)]^{-1}$ and $P''(v)$ (the Fréchet second derivative) are bounded in some neighbourhood $b(v^*,r)$, with $P(v^*) = 0$, then Linz [1979], p.148, shows the Newton-Kantorovich method has a second-order rate of convergence near v^*. However, under these conditions the modified form has only a first order rate of convergence. Due to the ill-posed nature of our problems generally $[P'(v)]^{-1}$ will not be bounded. However, this will hold for the regularized problem.

The Newton-Kantorovich method does not always converge. One possible method of increasing the region of convergence of the iteration is to use the damped form of Newton's method

$$v^{(k+1)} = v^{(k)} + \alpha^{(k)} s^{(k)}$$

where $\alpha^{(k)} \leq 1$ is chosen using a linesearch to minimize an appropriate functional. The quantity $s^{(k)}$ solves (1.12) as before.

The damped scheme will still fail if $[P'(v)]^{-1}$ is unbounded. An alternative is to use the Levenberg-Marquadt method where a bias towards steepest descent is added. This has the property of global convergence to a local minimizer of the functional being minimized. Daniel [1971] pp.190-193 and Fletcher [1980] Vol. 1, Chapter 6, contain further details of these extensions to Newton's method.

A practical implementation would generally include the use of regularization techniques (see §1.3.2). A scheme based upon Miller-Tikhonov regularization combined with the Marquadt-Levenberg method is outlined in Kristensson and Vogel [1986]. This is used to solve an inverse scattering problem.

We note here several authors use the Levenberg-Marquadt method itself to regularize the problem (see Coen *et al.* [1981]). Then the tuning parameter of the Levenberg-Marquadt method is varied to some non-zero value (which corresponds to the regularization parameter).

On the other hand, if the Tikhonov selection method is used to regularize the problem, a constrained optimization method is required. For example, the results in Colton [1984] are obtained with a procedure from Madsen and Schjaer-Jacobsen [1978] which is based upon Newton's method.

We note that in the above optimization methods a Gauss-Newton type approximation to the Hessian is used, namely

$$H^{(k)} \simeq P'(v^{(k)})^* P'(v^{(k)})$$

where the superscript '*' denotes the adjoint. The true Hessian is generally expensive to compute as it involves second derivative information (i.e. P'' must be found).

1.4.4 *Review of Iterative Methods*

The solution of inverse problems in general with the Newton-Kantorovich method was discussed in Connolly *et al.* [1985]. Backus and Gilbert [1967] seem to be the first authors to use the Newton-Kantorovich method to solve an inverse problem. They applied it to a problem of free oscillation of the Earth.

Time domain inverse problems for a coefficient in wave and diffusion equations have been solved with the Newton-Kantorovich method by Chen and Tsien [1977], Chen [1979], Chen and Liu [1981, 1982] and Hatcher and Chen [1983]. The Newton-Kantorovich and related methods have been applied to the reconstruction of spatially varying refractive indices in inverse scattering problems - see Tsien and Chen [1978], Roger [1978] and Coen *et al.* [1981].

The method has been applied to the determination of electrical conductivity, with imaging purposes in mind, by Connolly [1985], Murai and Kagawa [1985], Breckon and Pidcock [1986] and Connolly and Wall [1988].

Inverse boundary scattering problems have also been solved with the Newton-Kantorovich method and variants by Roger [1981], Colton [1984], Wall *et al.* [1985], Kristenssson and Vogel [1986] plus Murch, Tan and Wall [1988] (see also Tan [1988]).

However, most of the authors, unlike us, do not formally prove the Fréchet differentiability of their nonlinear operators before implementing the Newton-Kantorovich method. Also, a number of authors - Gray and Hagin [1982], Tijhuis [1981], Tijhuis and Van der Worm [1984] and Johnson and Tracy [1983a] for example - use iterative methods that are derived in an ad hoc manner to solve inverse scattering problems. These like the Newton-Kantorovich method (as shall be seen in the sequel) involve the solution of a first kind integral equation for the update at each operation - and so are obviously closely related. We shall show later that in fact a number of such schemes suggested in the literature are actually variants of the Newton-Kantorovich method.

Iterative schemes other than the Newton-Kantorovich method may be used to solve the nonlinear operator equation (1.3). Gradient methods such as steepest descent have been utilized to solve inverse problems by Weston [1979], Chavent [1983] and Lesselier [1982] for example. We examine such a scheme in §6.5. Also the method of inversion of power series (see Rall [1969]) may be used. This method has been applied to inverse scattering problems by Jost and Kohn [1952] and Prosser [1968, 1975, 1979] where it is known as inversion of Born series.

1.4.5 *Parameter Identification*

Another conceptually different way of solving the inverse problem is known as parameter identification. In this approach the solution of the inverse problem is expressed by a finite number of parameters. These parameters are to be determined as the solution to a nonlinear system of algebraic equations - see Parker [1977] for example. However, we shall see later that this approach is very closely related to the nonlinear operator method of solution outlined in this chapter.

The nonlinear equations are defined by requiring the solution of the corresponding direct problem to satisfy the measurements. We shall denote the vector of parameters to be determined by $\underline{a}$. Usually these will be the unknown coefficients in a basis function expansion for f. Let $y(\underline{a};\underline{x})$ be the solution of the direct problem with coefficient function given by $\underline{a}$. Define $\{\underline{x}_i\}$, $i \in \{1, \ldots, M\}$ as the set of points at which measurements are made. Denote these measurements by $\Sigma(\underline{x}_i)$. Then the nonlinear system of equations $\underline{r}(\underline{a}) = \underline{0}$ is

$$r_i(\underline{a}) = y(\underline{a};\underline{x}_i) - \Sigma(\underline{x}_i) = 0 \, , \; i \in \{1, \ldots, M\} \; . \tag{1.14}$$

For the inverse problem to be deterministic, N, the number of undetermined parameters in $\underline{a}$, is required to be less than or equal to the number of measurements, M. Thus if $N < M$ there is an overdetermined system to solve.

The system of nonlinear equations (1.14) may then be solved for $\underline{a}$ and hence f, by the Gauss-Newton method or its variants - see Fletcher [1979], Vol.1, Chapter Six, for example. The Gauss-Newton method for a system of nonlinear equations $\underline{r}(\underline{a}) = \underline{0}$ is the following iterative scheme

$$\underline{a}^{(k+1)} = \underline{a}^{(k)} + \underline{s}^{(k)}$$

where the update $s^{(k)}$ satisfies

$$J^{(k)}\underline{s}^{(k)} = -\underline{r}(\underline{a}^{(k)}) \quad . \tag{1.15}$$

$J^{(k)}$ is the Jacobian matrix of $\underline{r}(\underline{a})$ at the kth iteration. The Jacobian matrix is determined from the direct problem formulation. If N < M, then the overdetermined system (1.15) is solved in the least squares sense. The iterative scheme is then being used to minimize $\underline{r}^T\underline{r}$.

In practice the parameter set is often defined by dividing up the region on which the solution is defined into a number of subregions. The solution then has a constant value, which is to be determined on each of the subregions. This approach is very useful for approximating discontinuous media. Generally a canonical solution for the direct problem is then used in deriving the Jacobian matrix. However, this is not necessary as will be shown in Chapter 3 where the Gauss-Newton method for an interior measurement problem is derived.

The scheme outlined in this section is in fact related to the nonlinear operator approach in the following manner. Assume the same discretization is used to solve the linear operator equations resulting from the Newton-Kantorovich method as is used for the parameter identification. Then the resulting set of linear algebraic equations is the same as that obtained by using the Gauss-Newton method with parameter identification. Essentially this means that discretizing the problem then linearizing it gives the same result as linearizing it then discretizing - which is to be expected.

A proof of the result is to be found in Wouk [1979] p.312. This equivalence is illustrated with an example for an interior measurement inverse problem in Chapter 3.

1.5 THEORETICAL CONSIDERATIONS

In order for our nonlinear operator approach to succeed, the measurements must depend continuously upon the function we are trying to reconstruct. That is, the solution of the partial differential equation must depend continuously upon the coefficient function or boundary that is to be determined. The operator P(v) is then continuous. For example, if P is continuous from some space only into L^2, then there is no use in utilizing point measurements to reconstruct the function.

In addition the use of the linearization method (1.8) or the Newton-Kantorovich scheme (1.12) to solve the inverse problem, requires the nonlinear operator P(v) to be Fréchet differentiable. Also, for regularization purposes (see §1.4), P(v) must be a continuous operator. Continuity for its inverse may then be obtained.

We note that some authors have implemented iteration schemes claiming to be the Newton-Kantorovich method without proving the necessary Fréchet differentiability results. Also regularization techniques have been used without establishing continuity of the map and the compactness of their domain.

In this section we use the implicit function theorem to give sufficient conditions for the operator P(v) to be continuous or Fréchet differentiable - with Fréchet derivative (1.11). As shall be seen in later chapters, the sufficient conditions are applicable to the different problems that we consider. We shall also outline how Lipshitz continuity and compactness results may be proven for the operator.

1.5.1 *Review*

The implicit function theorem has been used to prove Fréchet differentiability results for several interior measurement problems by Chavent [1983] and Kravaris and Seinfeld [1985]. They consider inverse problems for elliptic and parabolic equations and use gradient methods to obtain equations.

We extend this approach so that it is applicable in more general situations such as exterior and boundary measurement inverse problems. Also, they only consider Hilbert spaces for the solutions of their partial differential equations. We consider solutions belonging to a range of different Banach spaces for a variety of problems. The versatility of this approach, via the implicit function theorem, for proving Fréchet differentiability and continuity, does not seem to have been appreciated in the literature where a variety of different techniques have been used to obtain such results.

The first work on proving Fréchet differentiability appears to have been in the geophysics literature. Woodhouse [1976] considered the expression for the Fréchet derivative of Backus and Gilbert [1968] for the inverse problem of free oscillation of the Earth. The Fréchet derivative was based upon a variational principle due to Rayleigh. Woodhouse showed that this was not valid for coefficient functions belonging to the space L^2 and with discontinuities present. However, as was pointed out by Parker [1977b], it was still possible that the Fréchet derivative was valid with a different choice of function space such as L^∞.

The difficulties with this particular problem (and a comment in Anderssen [1975]) motivated Parker [1977b] to examine the existence of the Fréchet derivative for an inverse scattering problem of a layered earth, derived in Parker [1970]. A Fréchet differentiability result is given however the methods used are not very rigorous.

In more recent times continuity and Fréchet differentiability results for various problems have appeared in the mathematical literature. Apart from the aforementioned work of Chavent and Kravaris and Seinfeld, the results have been proved directly without the use of the implicit function theorem.

Bamberger *et al.* [1979] show the Lipshitz continuity of the appropriate map for a one-dimensional wave equation. The compactness of their domain ensures the existence of the solution to the inverse problem formulated as a minimization problem. Numerical results from the use of a gradient method are given.

Symes [1983a] shows that the boundary values of the solution of the linear acoustic wave equation depend either Hölder or Lipshitz continuously upon a coefficient in the equation. In addition, Symes [1986] establishes Fréchet differentiability for the same problem, and the stability of the linearized problem is considered. We note Symes [1983b] gives an example where the appropriate map for this time domain problem is not Fréchet differentiable for some apparently natural choices of function spaces. The reader is referred to Symes [1986] for further discussion of such questions.

Some work has also been done on inverse boundary scattering problems. Colton and Kirsch [1981a] along with Angell *et al.* [1982] (see also Colton and Kress [1983] have shown that for an inverse boundary scattering problem the measured far-field pattern depends continuously upon the shape of the boundary. The first paper is concerned with the problem in two dimensions and the second the same problem in three dimensions. Colton and Kirsch [1981b] showed the far-field depends continuously upon an impedance boundary condition defined on a known boundary. These inverse problems are stabilized using ideas based upon the Tikhonov selection method. However, no Fréchet differentiability results are proven.

1.5.2 *Frechet Differentiability*

We shall show how the implicit function theorem may be utilized to prove continuity and Fréchet differentiability for the nonlinear operator P(v). First however we formally define these two properties.

Let P be a nonlinear operator mapping from E_1 into E_2, where E_1 and E_2 are two normed vector spaces. The operator, P, is continuous at the point $v_0 \in E_1$, if

$$\lim_{||v-v_0||_{E_1} \to 0} ||P(v) - P(v_0)||_{E_2} = 0 \tag{1.16}$$

The operator, P, is continuous, if it is continuous at every point of the space E_1.

The operator, P, is called Fréchet differentiable at a point v_0, if the increment $P(v_0 + \delta v) - P(v_0)$ can be expressed in the form

$$P(v_0 + \delta v) - P(v_0) = B\delta v + \omega(v_0, \delta v) .$$

Here B is a bounded linear operator mapping from E_1 into E_2, and $\omega(v_0,\delta v)$ is an operator satisfying the condition

$$\lim_{||\delta u||_{E_1} \to 0} \frac{||\omega(v_0, \delta v)||_{E_2}}{||\delta v||_{E_1}} = 0 . \tag{1.17}$$

The operator B is called the Fréchet derivative of P at the point v_0 and is denoted by $P'(v_0)$.

It should be noted that Fréchet differentiability at v_0 implies continuity at v_0 as

$$||P(v_0 + \delta v) - P(v_0)||_{E_2} \leq ||B|| \, ||\delta v||_{E_1} + ||\omega(v_0,\delta v)||_{E_2}$$

which tends to zero as $||\delta v||_{E_1}$ tends to zero.

We note here that the Fréchet second derivative, $P''(v)$ is a bilinear mapping on the cartesian product of the space E_1 with itself (see Wouk [1979] p.274 for a definition).

There is another possible definition for the derivative of an operator. Let $P: E_1 \rightarrow E_2$ be an operator between two normed vector spaces. If for $v_0 \in E_1$ there exists a linear operator $P_W'(v_0)$ such that for all $h \in E_1$

$$\lim_{s \to 0} \frac{P(v_0 + sh) - P(v_0)}{s} = P_W'(v_0)h \tag{1.18}$$

then we say P is weakly differentiable at v_0. The operator $P_W'(v_0)$ is called the weak or Gateaux derivative at v_0.

While there exists a close relationship between the two notions of differentiability, they are not equivalent. In particular, Fréchet differentiability at v_0 implies Gateaux differentiability at v_0 with $P_W'(v_0) = P'(v_0)$.

However, the converse is not true - an operator may have a weak derivative but not a strong one.

For the remainder of this thesis we shall generally only be interested in Fréchet differentiability - which is required to apply the Newton-Kantorovich method. However, to use a gradient method to minimize an appropriate functional (see §6.5), only Gateaux differentiability is required.

Given the formal definition of the Fréchet derivative from (1.7), the Newton-Kantorovich method may be derived by the following intuitive argument, analogous to that often used to derive Newton's method for solving nonlinear algebraic equations. Let v^* be a solution of $P(v) = 0$; then for v near v^*

$$0 = P(v^*) = P(v) + P'(v)(v^*-v) + \omega(v,v^*-v)$$

where ω is a small second term.

If $\omega(v,v^*-v)$ is neglected and what is left solved for v, the exact solution is not obtained, but hopefully a better approximation to it. This suggests the iterative process

$$v^{(k+1)} = v^{(k)} + s^{(k)} \tag{1.19}$$

where $s^{(k)}$ is a solution of the linear operator equation

$$P'(v^{(k)})\, s^{(k)} = - P(v^{(k)}) \ . \tag{1.20}$$

$P'(v^{(k)})$ is the Fréchet derivative of P at $v^{(k)}$.

1.5.3 *The Implicit Function Theorem*

We now investigate the application of the implicit function theorem. Let X,Y and W be Banach spaces, $\xi(v,y)$ a functional on $X \otimes Y$ with range in W. Suppose that there exists an open subset X_0 of X such that for every $v \in X_0$ the equation $\xi(v,y) = 0$ has one and only one solution $y = y(v) \in Y$. ξ_v and ξ_y shall denote partial Fréchet derivatives of ξ with respect to v and y. We then have

THEOREM 1.1 (Implicit function theorem)

(i) Assume for $v \in X_0$ and $y \in Y$

1. $\xi(v,y)$ is continuous.
2. $\xi_y(v,y)$ is continuous in v and y.
3. $[\xi_y(v,y)]^{-1}$ exists in $[W \rightarrow Y]$.

Then the map $v \rightarrow y(v)$ from $X_0 \rightarrow Y$ is continuous.

(ii) Moreover, if $\xi_v(v,y)$ is continuous in v and y then the map is Fréchet differentiable with

$$y'(v) = -[\xi_y(v,y)]^{-1}\xi_v(v,y) \quad .$$

<u>Proof</u> The theorem is proved (Wouk [1977] pp.294-297) by applying a contraction mapping theorem to the equation

$$y = \Phi(y)$$

where

$$\Phi(y) = y - \Gamma\xi(v,y)$$

and

$$\Gamma = [\xi_y(v_0,y(v_0))]^{-1} \quad .$$

This then gives existence of a solution and continuity of the map $v \to y(v)$ in a neighbourhood of some function v_0, for which there is a unique solution $y(v_0)$ to the direct problem. It also gives Fréchet differentiability at v_0.

Continuity and Fréchet differentiability on the whole of the open subset X_0 are then obtained from the existence of a unique solution $y(v)$ for any v belonging to X_0 (Schwartz [1967] pp.277-304). That is, the contraction mapping approach is applied at each $v_0 \in X_0$. □

The basic form of the implicit function theorem giving Fréchet differentiability at a particular $v_0 \in X_0$ is not strong enough for our purposes. In solving inverse problems we require Fréchet differentiability at all $v \in X_0$, thus the need for the wider form of the implicit function theorem in THEOREM 1.1.

For Fréchet differentiability of the map $v \to y(v)$, ξ is required to be continuously differentiable and also ξ_y^{-1} bounded. We note that if ξ is n times continuously differentiable, then the above implicit function theorem may be extended to show the map is in fact C^n (Schwartz [1967]).

The implicit function theorem gives Fréchet differentiability for the direct problem solution. Where this is the quantity measured, such as the interior measurement problems of Chavent [1983] and Kravaris and Seinfeld [1985], this is sufficient. However, for our purposes the following extension is needed.

COROLLARY 1.1

If $B(v,y)$ is continuously differentiable (has continuous partial derivatives) then $B(v,y(v))$ is Fréchet differentiable with respect to v. Moreover

$$B'(v) = B_v(v,y) + B_y(v,y)\, y'(v) \quad ,$$

where $y'(v)$ is given by THEOREM 1.1.

<u>Proof</u> This result follows from the chain rule (see Wouk [1979] p.300) and THEOREM 1.1. □

B_v and B_y denote the partial Fréchet derivatives of B with respect to v and y. This result is used when boundary measurements are utilized - then B is a trace operator. The corollary also allows for measurements of the derivatives of y and for cases where the measurements depend explicitly upon v as well as y, such as in our example (1.4).

To prove Fréchet differentiability results for our nonlinear operator formulation of the inverse problem, it is now clear we need existence, uniqueness, and regularity results for the direct problem. In particular, the third condition in the implicit function theorem is a fairly strong regularity result for the direct problem. It requires the solution of the direct problem (or its linearization if it is nonlinear) to depend continuously upon a source term in the equation.

So before we tackle each of the various inverse problems of this thesis, the properties of the associated direct problem are examined. Where the required regularity results are not available in the literature, these are proven.

In Chapter Three we use the implicit function theorem to obtain a Fréchet differentiability result for classical solutions of the steady-state diffusion equation. COROLLARY 1.1 is later utilized to extend this to the boundary measurement problem.

In Chapter Six several Fréchet differentiability results are proven for solutions of the Helmholtz equation with a spatially-varying refractive index. We also reconsider several existing continuous dependence results for boundary scattering problems via the implicit function theorem in Chapter Four.

1.5.4 *Lipschitz Continuity*

The implicit function theorem does not tell us the nature of the continuity obtained - whether it is Hölder continuous, Lipschitz continuous etc. We shall examine methods of establishing the Lipschitz continuity of the map.

A (nonlinear) operator $P: X \rightarrow Y$ is Hölder continuous with exponent α, $0 < \alpha \leq 1$, on $X_0 \subset X$ if there exists a constant K such that

$$||P(v_1) - P(v_0)||_Y \leq K||v_1 - v_0||_X^\alpha \quad \forall v_0 , v_1 \in X_0 .$$

If $\alpha = 1$ P is said to be Lipschitz continuous.

We have the following result for the Lipschitz continuity of P.

THEOREM 1.2 If X_0 is a convex subset of a Banach space and P is Fréchet differentiable and $\sup_{v \in X_0} ||P'(v)||_X$ exists then

$$||P(v_1) - P(v_0)||_Y \leq \sup_{v \in X_0} ||P'(v)|| \; ||v_1 - v_0||_X \quad \forall v_0 , v_1 \in X_0 .$$

Proof This follows from the mean-value theorem for operators (Wouk [1979] pp.265-266). □

So if it can be shown that our operator is Fréchet differentiable using the implicit function theorem or otherwise, and that the Fréchet derivative is bounded on a suitable subset X_0, then the map is Lipschitz continuous on X_0.

We shall also see that it is possible for several of our problems to prove directly this Lipschitz continuity result, without going via the implicit function theorem and Theorem 1.2. This gives us Lipschitz continuity on *bounded* subsets of X, i.e., $||v||_X \leq M$. This contrasts with an alternative approach used by both

Colton and Kress [1985] pp.242 and Weston [1979], which also does not utilize the implicit function theorem. Their method gives either Hölder or Lipschitz continuity but only upon compact subsets of X. The compactness assumption requires their functions to belong to a more regular space. For example, a Hölder continuous function may then be required for the solution rather than one belonging to L^{∞}.

We note that such Lipschitz continuity results provide a bound on the change in the direct problem solution (and hence the measurements) that results from a perturbation in the coefficient function, v. General stability results of this form for the inverse map would also be very useful.

1.5.5 *Compactness*

Let X, Z be normed spaces and P an operator from X into Z. A bounded set in a normed space is one which is contained in the ball $B_R(0)$ for some R. The operator P is called bounded if it maps bounded sets in X to bounded sets of Z. P is compact if it maps bounded sets in X to relatively compact sets of Z.

Every compact operator is bounded. For linear operators boundedness is equivalent to continuity.

Boundedness and compactness may also be defined on subsets of X. P is bounded on $X_0 \subset X$ if it maps bounded sets in X_0 to bounded sets of Z and similarly for compactness.

We shall outline one method for showing the compactness of our nonlinear operator. The function $y(v) \in Y$ is generally the solution of a partial differential equation and so Y is usually a space involving derivatives of y. However, the measurements will belong to a much less regular space than Y - such as L^2 for example. This measurement space will be denoted by Z.

THEOREM 1.3

If the operator $P: X \to Y$ is bounded and the imbedding $Y \to Z$ is compact, then

(i) $P: X \to Z$ is compact.

(ii) P cannot have a continuous inverse if X is infinite dimensional.

Proof (i) $P: X \to Y$ maps bounded sets in X to bounded sets in Y. However as the imbedding $Y \to Z$ is compact, bounded sets in Y are relatively compact in Z. So $P: X \to Z$ maps bounded sets to relatively compact sets as required.

(ii) Assume $P^{-1}: Z \to X$ was continuous and consider the composition $P^{-1}P = I$, the identity operator in the infinite-dimensional space X.

From (i) P maps bounded sets in X to relatively compact sets of Z. P^{-1} being continuous maps relatively compact sets of Z to relatively compact sets of X. The composition $P^{-1}P$ and hence the identity operator would then be compact. But this is impossible for X infinite dimensional. □

This result gives us compactness of nonlinear operator $P(v)$ if the space the direct problem solution belongs to, Y, is compactly imbedded in the measurement space Z. This also requires a boundedness result for P. Such a result is often available from regularity theory for the direct problem solution. Then if the space for the inverse problem solution, X, is infinite dimensional, then $P^{-1}: Z \to X$ (if it exists) is continuous. Thus small changes in the measurement data may cause arbitrarily large changes in the solution. Thus the inverse problem is ill-posed as it stands.

We prove such a result for the interior measurement version of the inverse problem of steady-state diffusion in Chapter Three. Here if the coefficient function, f, is Hölder continuously differentiable, then the solution, ϕ, of the direct problem (a second-order elliptic p.d.e. on Ω) is twice continuously differentiable, i.e. $Y = C^2(\overline{\Omega})$. So it follows that if point measurements of ϕ are utilized (i.e. $Z = C^0(\overline{\Omega})$) or distributed measurements used ($Z = L^2(\Omega)$) then the resulting nonlinear operator is compact.

The use of regularization techniques is then necessary to solve the inverse problem in the presence of measurement noise. Such a result is also given for the problem of Chapter Six - determining a refractive index of an object from point measurements of the scattered field external to the object.

We note here that THEOREM 1.3 may also be applied to the Fréchet derivative $P'(v)$ - a linear operator and bounded by definition. Alternatively, the Fréchet derivative of a compact operator is also a compact operator - see Nashed [1971]. However, the analogous result going the other way does not always hold.

It should also be noted that our nonlinear operators shall generally be completely continuous (that is, both continuous and compact) with the continuity following from the implicit function theorem or by other means.

If our nonlinear operator is compact, the solution of both the inverse problem and its linearization will not depend continuously upon the measurements. When a numerical solution of the compact operator equation is attempted, this manifests itself in highly oscillatory solutions.

In order to guarantee both the existence and stability of a solution to the inverse problem, it must be reformulated using regularization methods. These were outlined in §1.3.2. We give here an existence result for the Tikhonov selection method. This is from Colton and Kress [1983] pp.137-238.

THEOREM 1.4

Suppose $P(v)$: $X \to Z$ (X and Z are Banach spaces) is continuous, then there exists a solution to the problem

$$\min_{v \epsilon X_1} C(v) = \min_{v \epsilon X_1} ||P(v)||_Z$$

where $X_1 \subset X$ is compact.

<u>Proof</u> $P(v)$ is continuous so that $||P(v)||_Z$ is a continuous functional. It is a standard result that there exists a solution to the minimization of a continuous functional $C(v)$ over a compact set, however we include the proof here for completeness.

Let $\{v_n\}$ be a minimizing sequence, that is, $\lim_{n\to\infty} C(v_n) = \inf_{v\in X_1} C(v)$. Since X_1 is compact there exists a convergent subsequence $\{v_{n(j)}\}$ such that $v_{n(j)} \to v^*$ where $v^* \in X_1$. From the continuity of C it follows that $C(v^*) = \inf_{v\in X_1} C(v)$, that is, v^* is a solution to the minimization problem. □

Colton and Kress also give a continuous dependence result for the solution of this regularized problem upon the measurement data. See §1.3.2 for an outline of the statement of their theorem.

1.5.6 *Summary*

Much of this thesis is concerned with proving theoretical results relating to the solution of inverse problems. We summarize here reasons for this and also the means for proving such results. However, the final aim is obtaining a practical algorithm for the solution of such problems.

Firstly, for our nonlinear operator approach to be valid the measurements must depend continuously upon the function to be reconstructed. That is, the nonlinear operator should be continuous.

Moreover, to use the Newton-Kantorovich method to solve the nonlinear operator equation, it must be Fréchet differentiable. Both continuity and Fréchet differentiability are given by the implicit function theorem. The nature of the continuity, i.e., Lipschitz continuity, may be obtained via the mean value theorem for operators. We note that if it is only possible to prove Gateaux differentiability (a weaker condition than Fréchet differentiability) a gradient method must then be used to minimize an appropriate functional - rather than use the Newton-Kantorovich method.

In addition if it can be shown the operator or its Fréchet derivative is compact, then we know the solution of the inverse problem or its linearization is an ill-posed problem. That is, the solution does not depend continuously upon the measurement data. Then the use of regularization techniques is required. For these the solution is restricted to belong to a compact subset to ensure existence and stability. This also requires continuity of the operator formulation.

In some cases it is possible to show compactness of the operator when the measurement space is less regular than the space for the direct problem solution. Such a result first requires boundedness of the map. This is usually available from regularity theory for the direct problem solution.

We may summarize the approach to solving the inverse problem outlined in this chapter with the following flow diagram (Table 1.1).

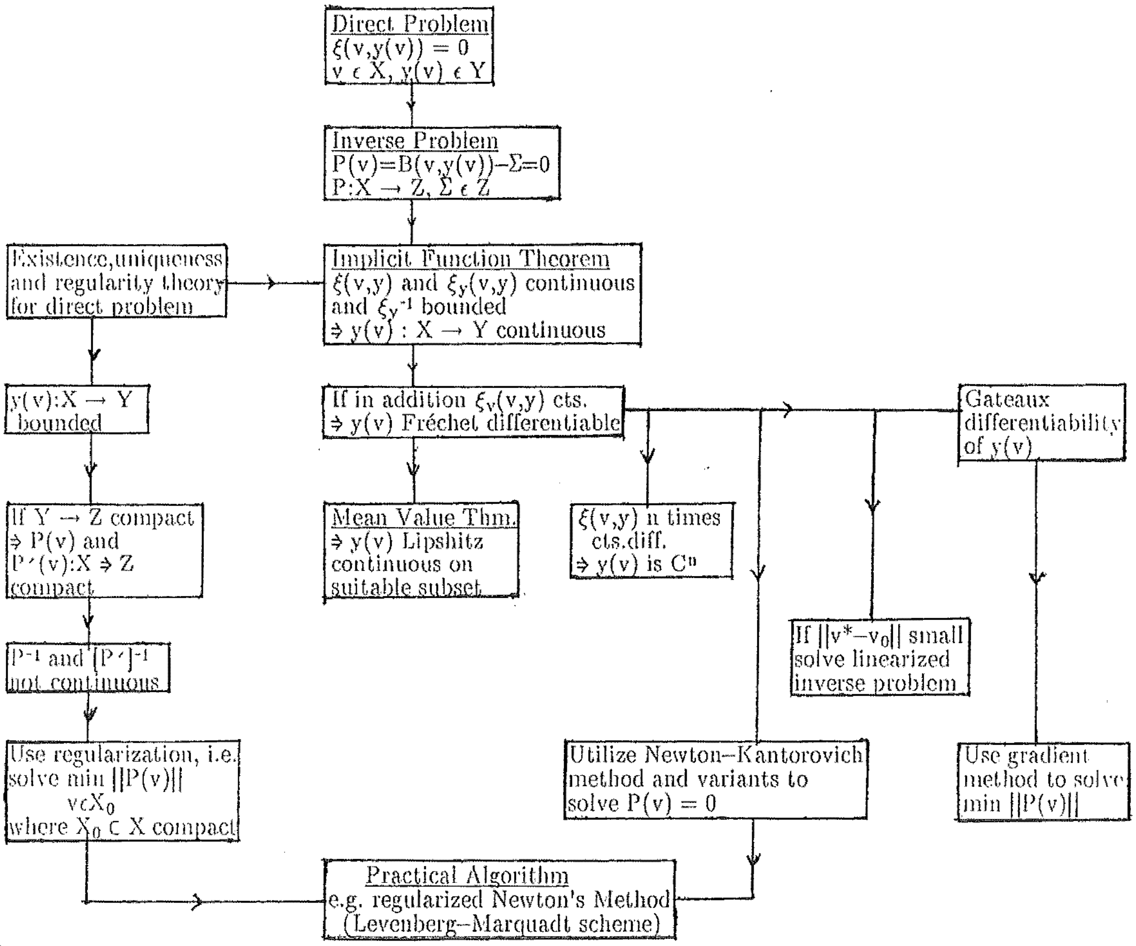
Direct Problem
ξ(v,y(v)) = 0
v ε X, y(v) ε Y
Inverse Problem
P(v)=B(v,y(v))−Σ=0
P:X → Z, Σ ε Z
Existence,uniqueness and regularity theory for direct problem
Implicit Function Theorem
ξ(v,y) and ξy(v,y) continuous and ξy-1 bounded
⇒ y(v) : X → Y continuous
y(v):X → Y bounded
If in addition ξv(v,y) cts.
⇒ y(v) Fréchet differentiable
Gateaux differentiability of y(v)
If Y → Z compact
⇒ P(v) and P′(v):X ⇒ Z compact
Mean Value Thm.
⇒ y(v) Lipshitz continuous on suitable subset
ξ(v,y) n times cts.diff.
⇒ y(v) is Cn
If ||v*−v0|| small solve linearized inverse problem
P-1 and [P′]-1 not continuous
Use regularization, i.e. solve min ||P(v)|| vεX0 where X0 ⊂ X compact
Utilize Newton–Kantorovich method and variants to solve P(v) = 0
Use gradient method to solve min ||P(v)||
Practical Algorithm
e.g. regularized Newton's Method (Levenberg–Marquadt scheme)

Table 1.1

CHAPTER TWO

STEADY-STATE DIFFUSION EQUATION

2.1 INTRODUCTION

Associated with the partial differential equation (p.d.e)

$$\nabla \cdot (f \nabla \phi) = \rho \ , \underline{x} \in \Omega \subset \mathbb{R}^n \tag{2.1}$$

(where Ω is a bounded domain) there are several problems. The first is the direct problem where given $f > 0$, ρ and appropriate boundary conditions on ϕ, the self-adjoint elliptic p.d.e. (2.1) is to be solved for ϕ.

The second problem is the inverse or identification problem, where given the p.d.e. (2.1), the source term ρ and boundary conditions on ϕ, the function f is to be determined from measurements of ϕ.

These measurements are made either

(i) in Ω or

(ii) on the boundary $\partial\Omega$ only.

In Chapter Three an inverse problem for steady-state diffusion which is of type (i) is considered. In the Appendix an inverse problem of type (ii) is examined where the electrical conductivity of a region is to be determined. Both of these problems are based upon the p.d.e. (2.1).

Two types of boundary conditions on ϕ shall be used. Firstly, Dirichlet conditions where ϕ is specified on $\partial\Omega$, and also Neumann conditions where $\frac{\partial \phi}{\partial n}$ is specified on $\partial\Omega$, and ϕ is given at one point of $\overline{\Omega}$. This last condition is necessary as without it the solution of the Neumann problem can only be unique up to an additive constant (i.e. constant functions are in the null space of the operator equation). As we shall only consider cases where $f > 0$, for Neumann conditions equivalently $f\frac{\partial \phi}{\partial n}$ may be specified on $\partial\Omega$, which makes more sense physically - this corresponds to the flow/current across the boundary.

To ensure the existence of a solution, the data must lie in the range of the operator. Hence for Neumann boundary conditions we have the solvability condition,

$$\int_{\partial\Omega} f\frac{\partial \phi}{\partial n}\,dS = \int_{\Omega} \rho\,dV. \tag{2.2}$$

This follows from integrating the p.d.e. (2.1) over Ω and then using the divergence theorem. The consistency condition has a simple meaning in steady-state heat conduction for example. This is that the steady-state can only be achieved if the net heat input from body sources is equal to the net heat flow through the boundary.

The direct problem for (2.1) has applications in a variety of areas of physics. These include electrostatics, magnetostatics, direct or low frequency electric current flow, irrotational fluid flow, steady-state heat flow, and fluid and molecular diffusion.

We will be examining inverse problems in steady-state diffusion and electric current flow. However, it is very likely that similar inverse problems in these other areas are of interest as well.

In this chapter we outline some properties of the direct problem. Extensive use of these is made in the following chapter on the inverse problems.

2.2 CLASSICAL SOLUTIONS

In this section we consider some properties of classical solutions to the partial differential equation (2.1) - that is, where f is continuously differentiable and the solution ϕ twice continuously differentiable.

2.2.1 *Integral Representations*

Firstly the following generalization of Green's theorems is useful in the study of both the direct and inverse problems. The generalization of Green's first theorem (Williams [1980], pp.127-128) is

$$\int_{\Omega} \phi_1 \nabla \cdot (f \nabla \phi_2) dV = \int_{\partial\Omega} f \frac{\partial \phi_2}{\partial n} \phi_1 dS - \int_{\Omega} f \nabla \phi_1 \cdot \nabla \phi_2 dV \,. \tag{2.3}$$

From this the generalization of Green's second theorem easily follows

$$\int_{\Omega} [\phi_1 \nabla \cdot (f \nabla \phi_2) - \phi_2 \nabla \cdot (f \nabla \phi_1)] dV = \int_{\partial\Omega} f(\phi_1 \frac{\partial \phi_2}{\partial n} - \phi_2 \frac{\partial \phi_1}{\partial n}) dS \,.$$

We require $f, \phi_1 \epsilon C^1(\Omega) \cap C^0(\overline{\Omega})$ and $\phi_2 \epsilon C^2(\Omega) \cap C^1(\overline{\Omega})$ for the first theorem, $f \epsilon C^1(\Omega) \cap C^0(\overline{\Omega})$ and $\phi_1, \phi_2 \epsilon C^2(\Omega) \cap C^1(\overline{\Omega})$ for the second theorem (John [1978], p.64).

Using these Green's theorems we may derive an integral representation for the solution of the Dirichlet direct problem (Williams [1980], pp.131-133). If (2.1) is satisfied and

$$\phi = g \text{ on } \partial\Omega$$

then

$$\phi(\underset{\sim}{x}) = \int_{\Omega} G_1(\underset{\sim}{x}, \underset{\sim}{x}') \rho(\underset{\sim}{x}') dV' + \int_{\partial\Omega} f \frac{\partial G_1}{\partial n'} g \, dS' \,. \tag{2.4}$$

$G_1(\underline{x},\underline{x}')$ is a Green function and satisfies

$$\nabla \cdot [f(\underline{x}')\nabla' G_1(\underline{x},\underline{x}')] = \delta(\underline{x}' - \underline{x}) \tag{2.5}$$

and

$$G_1(\underline{x},\underline{x}') = 0 \quad \text{when } \underline{x}' \epsilon \partial\Omega \ .$$

Here ∇' and $\nabla' \cdot$ denote the gradient and divergence with respect to the primed variables.

For the Neumann problem, a modified Green function, G_2, must be used so that the consistency condition (2.2) is satisfied. Thus

$$\nabla' \cdot [f(\underline{x}')\, \nabla' G_2(\underline{x},\underline{x}')] = \delta(\underline{x}' - \underline{x}) - 1/(\int_\Omega dV') \ ,$$

$$f \frac{\partial G_2}{\partial n'}(\underline{x},\underline{x}') = 0 \quad \text{when } \underline{x}' \epsilon \partial\Omega \tag{2.6}$$

and

$$\int_\Omega G_2(\underline{x},\underline{x}')\, dV' = 0 \ .$$

This last condition is imposed so that the Green function is uniquely defined. If the p.d.e. (2.1) is satisfied and

$$f \frac{\partial \phi}{\partial n} = h \quad \text{on } \partial\Omega$$

then

$$\phi(\underline{x}) = \int_\Omega G_2(\underline{x},\underline{x}')\rho(\underline{x}')dV' - \int_{\partial\Omega} G_2 h dS' + \text{constant} \ . \tag{2.7}$$

The arbitrary constant may be determined from knowledge of ϕ at some point of $\overline{\Omega}$.

The Green functions G_1 and G_2 have a singularity at $\underline{x} = \underline{x}'$.

Williams [1980] pp.132-133, shows that for $\underset{\sim}{x} \in \mathbb{R}^2$, near $\underset{\sim}{x} = \underset{\sim}{x}'$

$$G_1, G_2 \approx \frac{1}{2\pi f(\underset{\sim}{x})} \log |\underset{\sim}{x} - \underset{\sim}{x}'|$$

and $\underset{\sim}{x} \in \mathbb{R}^3$

$$G_1, G_2 \approx \frac{1}{4\pi f(\underset{\sim}{x})} |\underset{\sim}{x} - \underset{\sim}{x}'|^{-1} .$$

2.2.2 *Existence and Uniqueness*

For the case where f is Hölder continuously differentiable and ϕ twice Hölder continuously differentiable, existence and uniqueness results have been proved - see Courant and Hilbert [1962], Vol. 2, pp.331-341 for Dirichlet boundary conditions. We shall outline one of the results here. The analogous result for an oblique derivative boundary condition is to be found in Gilbarg and Trudinger [1983], p.128.

The domain Ω is required to be convex and smooth (i.e. $C^{2,\alpha}$). The definition of a smooth domain is analogous to that for a C^{∞} domain contained in the next section. We consider the Dirichlet problem

$$\begin{aligned} \nabla\cdot(f\nabla\phi) &= \rho \ , \ \underset{\sim}{x} \in \Omega \\ \phi &= g \ , \ \underset{\sim}{x} \in \partial\Omega \ . \end{aligned} \tag{2.8}$$

THEOREM 2.1 For $f \in C^{1,\alpha}(\overline{\Omega})$ with $f > 0$, $\rho \in C^{0,\alpha}(\overline{\Omega})$ and $g \in C^{2,\alpha}(\partial\Omega)$ there exists a unique solution $\phi \in C^{2,\alpha}(\overline{\Omega})$ to (2.8).

Moreover

$$||\phi||_{2,\alpha} \leq K(f,\Omega)(||\rho||_{0,\alpha} + ||g||_{2,\alpha}) \ .$$

Proof The Courant and Hilbert result is for the more general equation

$$\sum_{i,k=1}^{n} a_{ik}\phi_{ik} + \sum_{i=1}^{n} b_i\phi_i + c\phi = \rho \ .$$

Our equation is on expanding (2.1)

$$\sum_{i,k=1}^{n} f\phi_{ik} + \sum_{i=1}^{n} f_i\phi_i = \rho \ .$$

For their result Courant and Hilbert require the a_{ik}, b_i and c to belong to $C^{0,\alpha}(\overline{\Omega})$. The imbedding $C^{1,\alpha}(\overline{\Omega}) \to C^{0,\alpha}(\overline{\Omega})$ is bounded (see Adams [1975] pp.10-11 for example). It then follows that if $f \in C^{1,\alpha}(\overline{\Omega})$ then f and f_i, i = 1, .., N belong to $C^{0,\alpha}(\overline{\Omega})$ and the Courant and Hilbert result is applicable. Their result is proven by using the method of continuity to reduce the problem to Poisson's equation.

□

Similar results for less smooth domains can also be found in Courant and Hilbert.

2.2.3 *Piecewise Differentiable Coefficient*

If the function f is piecewise continuously differentiable with smooth interfaces between the regions on which f is C^1, then the direct problem may be solved as follows. The differential equation is satisfied on each of the regions and continuity of the potential, ϕ, and the normal "current", $f\,\frac{\partial\phi}{\partial n}$, is required across the interfaces - see Stakgold [1968], Vol. 2, pp.183-185, for instance. However, if the interfaces are not smooth, then possible singularities at the corners of the interfaces have to be taken into account - see Babuska and Aziz [1972] pp.280-281.

These jump conditions along with their relationship with the weak solutions introduced in the next sub-section, are discussed in more detail in §4.2.

2.3 WEAK SOLUTIONS

In this section we consider weak solutions of our partial differential equation - where $f \notin C^1(\Omega)$ and $\phi \notin C^2(\overline{\Omega})$. In what follows the function f is to be bounded below by a constant greater than zero.

Case 1. Dirichlet boundary conditions.

Consider the elliptic p.d.e.

$$\nabla\cdot(f\nabla\phi) \overset{w}{=} \rho \ , \ \underset{\sim}{x} \in \Omega \subset \mathbb{R}^n \ ;$$
$$\phi = g \ , \ \underset{\sim}{x} \in \partial\Omega \ . \qquad (2.9)$$

The differentiations in (2.9) are to be interpreted in the sense of distributions. We require $f \in L^{\infty}(\Omega)$, $\rho \in H^{-1}(\Omega)$ and $g \in H^{\frac{1}{2}}(\Omega)$. Then it follows (see Oden and Reddy [1979], Chapter Seven, for example) that the problem of finding $\phi \in H^1(\Omega)$ such that (2.9) holds is equivalent to the following variational boundary-value problem.

Find $\phi \in H^1(\Omega)$ with $\phi = g$ on $\partial\Omega$ such that

$$\int_\Omega f\nabla\phi\cdot\nabla v \, dV = \int_\Omega \rho v \, dV \qquad \forall v \in H_0^1(\Omega) \ . \qquad (2.10)$$

Case 2. Neumann boundary conditions.

Consider

$$\nabla\cdot(f\nabla\phi) \overset{w}{=} \rho \ , \underset{\sim}{x} \in \Omega \subset \mathbb{R}^n \ ;$$

$$\frac{\partial\phi}{\partial n} = h \ , \underset{\sim}{x} \in \partial\Omega \ . \tag{2.11}$$

We require $f \in L^{\infty}(\partial\Omega)$, $\rho \in H^{-1}(\Omega)$ and $h \in H^{-\frac{1}{2}}(\partial\Omega)$. Then the problem of finding $\phi \in H^1(\Omega)$ such that (2.1) holds is equivalent to the following variational problem.

Find $\phi \in H^1(\Omega)$ such that

$$\int_{\Omega} f\nabla\phi\cdot\nabla v \, dV - \int_{\partial\Omega} fhv \, dS = \int_{\Omega} \rho v \, dV \quad \forall v \in H^1(\Omega) \ . \tag{2.12}$$

We quote existence, uniqueness and regularity results for the variational boundary value problems just outlined. For these we require Ω to be a C^{∞} domain (this may be relaxed - see the Appendix). The boundary of a C^{∞} domain may be covered by a finite number of spheres with the property that, singling out one co-ordinate, say x_n, one can express the part of the boundary contained in each of these spheres in the form

$$x_n = y(x_1, x_2, \ldots, x_{n-1}) \ ,$$

where the function y has derivatives of all orders.

For the Dirichlet problem we have the result.

THEOREM 2.2 For $f \in L^{\infty}(\Omega)$ with $f > 0$, $\rho \in H^{-1}(\Omega)$ and $g \in H^{\frac{1}{2}}(\partial\Omega)$ there exists a unique solution, $\phi \in H^{1}(\Omega)$, to (2.9).

Moreover

$$||\phi||_{H^1(\Omega)} \leq C_1(f,\Omega)(||\rho||_{H^{-1}(\Omega)} + ||g||_{H^{\frac{1}{2}}(\Omega)}) .$$

Proof Follows from the standard weak theory for partial differential equations - see Tréves [1975]. □

For the Neumann problem we have

THEOREM 2.3 For $f \in L^{\infty}(\Omega)$ with $f > 0$, $\rho \in H^{-1}(\Omega)$ and $h \in H^{-\frac{1}{2}}(\Omega)$ there exists a solution $\phi \in H^{1}(\Omega)$ to (2.11), unique up to an additive constant.

Moreover

$$||\phi||_{\overset{o}{H}{}^1(\Omega)} \leq C_2(f,\Omega)(||\rho||_{H^{-1}(\Omega)} + ||h||_{H^{-\frac{1}{2}}(\partial\Omega)}) .$$

Here $\overset{o}{H}{}^1(\Omega)$ is the quotient space $H^1(\Omega)$, modulo the constant functions.

Proof Again follows from the standard weak theory. □

We note here that this weak theory is the basis of the finite element method for numerical solution of elliptic partial differential equations - see Mitchell and Wait [1977]. The finite element method uses piecewise polynomial trial spaces to obtain solutions. For a description of finite difference methods of solution to the self-adjoint elliptic p.d.e. (2.1) the reader is referred to Mitchell and Griffiths [1980] p.114-117. Such numerical methods for the solution of the equation are necessary with arbitrary coefficient function, f.

In the following chapter inverse problems for the equation (2.1) are considered. It is mainly concerned with the interior measurement problem but a boundary measurement problem is also considered. The boundary measurement problem is considered in more depth in the Appendix.

Applied to the inverse problems the weak theory allows the reconstruction of discontinuous functions while the classical theory gives more regularity for the direct problem solution allowing the use of point measurements for example. Also within the classical theory an explicit expression involving a Green function may be derived for the Fréchet derivative of the map $f \rightarrow \phi(f)$.

For reasons that will become apparent later, we concentrate on the use of the classical regularity theory for the interior measurement problem and the weak theory for the boundary measurement problem.

CHAPTER THREE

AN INTERIOR MEASUREMENT PROBLEM

3.1 INTRODUCTION

The inverse problem considered in this chapter has applications in the study of ground water flow and oil reservoirs. The model equation is the steady-state diffusion equation, previously considered in Chapter Two for the direct problem

$$\nabla \cdot (f \nabla \phi) = \rho \ , \ \underline{x} \in \Omega \subset \mathbb{R}^n \tag{3.1}$$

with appropriate boundary conditions on ϕ, where Ω is a bounded domain. Here ϕ represents pressure or "piezometric head", ρ is a source term, and f is a positive function often referred to as the "transmissivity" or diffusion coefficient.

The identification of the spatially varying f is required, using measured ϕ and ρ values at well sites - see the review by Yeh [1986]. These measurements are available at a finite number of points in Ω. We note that this interior measurement inverse problem has a different character from the boundary measurement problem considered in §3.6 and the Appendix. This problem is somewhat easier to solve, however there are similarities in the method of solution we employ in each case.

In this chapter we first consider the direct identification of the diffusion coefficient by solving (3.1) for f. The uniqueness and continuous dependence of the solution upon the measurements for the inverse problem are then reviewed.

The indirect or parameter identification approach to this inverse problem is also considered. Here f is solved for in an iterative manner. A new approach to the problem using the Newton-Kantorovich method is derived. This gives an integral equation to solve at each iteration for the update on f. We also derive a much tidier formulation of the Gauss-Newton method for parameter identification than that used by previous authors. The advantages of indirect over direct methods are discussed at the end of §3.2.

In §3.3 a one-dimensional problem is examined in more detail and numerical results from its solution are presented in §3.4.

A Fréchet differentiability result for this inverse problem is proven in §3.5. A compactness result is also obtained for the nonlinear operator and regularization methods for the solution of the inverse problem investigated.

3.1.1 *Direct Identification*

One approach to identifying f is the "direct" one. If the functions ϕ and ρ are known on all of Ω, then we may solve the following first order linear hyperbolic equation for f

$$f\nabla^2\phi + \nabla f \cdot \nabla\phi = \rho \ . \tag{3.2}$$

This equation results from expanding (3.1).

If the condition $\inf_\Omega |\nabla\phi| > 0$ is satisfied, then (3.2) is a standard hyperbolic problem with non-intersecting characteristic traces. These traces are given by

$$\frac{d\underline{x}}{ds} = \frac{\nabla\phi}{|\nabla\phi|} \tag{3.3}$$

and a well-defined trace passes through each point of Ω. Richter [1981a] shows each trace must have finite length, and hence they must originate and terminate on the boundary. See Figure 3.1. The condition $\inf_\Omega |\nabla\phi| > 0$ is a physical hypothesis requiring some flow at each point of Ω.

This gives us a sufficiency condition for a unique solution to the hyperbolic equation. That is, f must be known along a surface crossed by all the characteristics passing through Ω. For example, knowing f along either the inflow or outflow portions of the boundary would be sufficient.

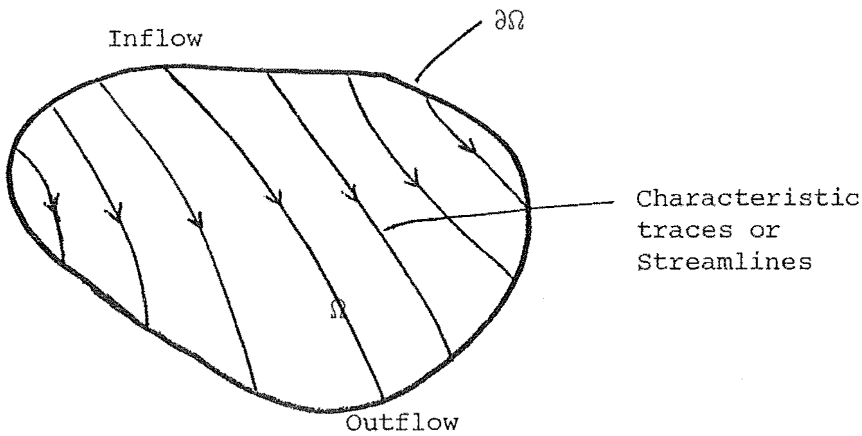

Figure 3.1

From the analytic solution of the hyperbolic equation (3.2), Richter [1981a] derives the following continuous dependence result for the inverse problem.

Let the function ϕ_1 satisfy $\inf_\Omega |\nabla\phi_1| > 0$. Also let f_1 be the corresponding diffusion coefficient and the source term be ρ_1. Thus

$$\nabla\cdot(f_1\nabla\phi_1) = \rho_1 \ .$$

Now suppose

$$\nabla\cdot(f_2\nabla\phi_2) = \rho_2 \ ,$$

where f_2 is the diffusion coefficient produced by a perturbed forward solution $\phi_2 \approx \phi_1$ and source function $\rho_2 \approx \rho_1$. Then if $f_1 = f_2$ on the inflow boundary which is determined by $\nabla\phi_1$, Richter shows

$$||f_1\text{-}f_2||_\infty \leq C_1||\Delta(\phi_1\text{-}\phi_2||_\infty + C_2||\nabla(\phi_1\text{-}\phi_2)||_\infty + C_3||\rho_1\text{-}\rho_2||_\infty \quad . \tag{3.4}$$

Here the quantities C_i are dependent upon the functions ϕ_1 and f_2.

This bound describes the sensitivity of f with respect to changes in the data, ϕ and ρ. It suggests that successful identification of f is possible only if the observed ϕ is precise enough to permit accurate approximation of the second derivatives of ϕ.

However, some knowledge of f is not necessary for a unique solution to the inverse problem under the following conditions. Consider the Neumann boundary condition on ϕ

$$f(\underline{x})\,\frac{\partial\phi}{\partial n}(\underline{x}) = h(\underline{x}) \quad \text{for} \quad \underline{x} \in \partial\Omega \ . \tag{3.5}$$

Also assume there exists a constant unit vector $\vec{\nu}$ and a constant σ such that

$$\nabla\phi\cdot\vec{\nu} \geq \sigma > 0 \quad \forall\underline{x} \in \partial\Omega \ . \tag{3.6}$$

This is a physical hypothesis stating that there is always some flow in the $\vec{\nu}$ direction. It is a stronger condition than $\inf_\Omega|\nabla\phi| > 0$.

Consider the following variational form of the p.d.e. (3.1) with the Neumann boundary conditions (3.5)

$$\int_\Omega f\,\nabla v\cdot\nabla\phi\, dV = \int_\Omega v\rho\, dV + \int_{\partial\Omega} hvdS \ . \tag{3.7}$$

This variational equation is of the same form as (2.11) for the direct problem. However in this context its solution, f, is a weak solution of the hyperbolic problem rather than the elliptic equation for ϕ.

Then under the conditions (3.6), Falk [1983] shows that if $\phi \in W^{2,\infty}(\Omega)$ then there is at most one $f \in H^1(\Omega)$ satisfying the variational equation (3.7). It is possible to get this uniqueness result as the Neumann boundary conditions (3.5) provide information for f on the boundary, which of course is not the case with Dirichlet conditions.

The uniqueness and continuous dependence of this inverse problem are established under conditions where $\nabla\phi$ is allowed to vanish, in Richter [1981a].

An approximation scheme using Galerkin's method for solving the hyperbolic problem was proposed in Frind and Pinder [1973]. This solves the variational equation (3.7) and so does not require explicit approximation of ∇f and $\Delta\phi$. A finite difference scheme for the hyperbolic equation (3.2) is given in Richter [1981b].

3.2 ITERATIVE METHODS

Often in practice there are insufficient measurements of ϕ to use the direct approach described in the previous section. This is because the coefficients of the hyperbolic equation which is solved involve derivatives of the measured quantity ϕ, see Richter [1981a]. Hence a common identification strategy is the "indirect" one in which one minimizes via an iterative process the deviation between a computed forward solution and the observations of ϕ.

This nonlinear optimization approach is equivalent to the parameter identification method outlined in the first chapter. There we formulated an arbitrary inverse problem as a system of nonlinear algebraic equations by requiring the computed forward solution to match the observations of ϕ. For the identification problem of this chapter, gradient methods such as steepest descent have been used to obtain solutions - see Chavent [1973]. Falk [1983] provides error estimates for such indirect identification schemes.

In this section the Newton-Kantorovich method is derived for indirect identification of this problem. Yeh and Yoon [1981], and also Sadeghipour and Yeh [1984], use a Gauss-Newton method on the parabolic (time-varying) form of the identification problem. We also derive a Gauss-Newton method for our problem. This approach is tidier than that of Yeh and Yoon, in that it does not require discretization of the problem to the same extent in computing equations satisfied by the Jacobian elements.

In addition it is shown that when the linear operator equations which are to be solved in the Newton-Kantorovich method are discretized in a certain manner, the resultant updates are the same as those produced by the Gauss-Newton method.

3.2.1 *Newton–Kantorovich Method*

We now formulate the Newton-Kantorovich method to solve the inverse problem. This is an indirect approach to identification of the coefficient function. Measurements, $\Phi(\underline{x})$, are made of ϕ so that the operator equation to be solved is

$$T(f) = \phi(f;\underline{x}) - \Phi(\underline{x}) = 0 \ , \ \underline{x} \in \Omega \ . \tag{3.8}$$

Here $\phi(f;\underline{x})$ is the solution of the direct problem (3.1) for a given coefficient f.

The Newton-Kantorovich method is the following iterative scheme

$$f^{(k+1)} = f^{(k)} + s^{(k)}$$

where the update $s^{(k)}$ satisfies

$$T'(f^{(k)})s^{(k)} = - T(f^{(k)}) \quad .$$

From (3.8) $T'(f)s = \phi'(f)s$. This Fréchet differential of the function ϕ is computed from the direct problem formulation

$$\nabla \cdot [f\nabla\phi(f)] = \rho \quad .$$

Differentiating with respect to f gives

$$\nabla \cdot [f\nabla\phi'(f)s] + \nabla \cdot [s\nabla\phi(f)] = 0$$

or

$$\nabla \cdot [f\nabla\phi'(f)s] = - \nabla \cdot [s\nabla\phi(f)] \quad . \tag{3.9}$$

We consider two different types of boundary conditions.

CASE 1

Dirichlet boundary conditions :

$$\phi(f) = g \ , \ \underset{\sim}{x} \in \partial\Omega \quad .$$

This gives

$$\phi'(f)s = 0 \ , \ \underset{\sim}{x} \in \partial\Omega \quad .$$

Thus the Fréchet differential satisfies homogeneous Dirichlet boundary conditions. Equation (3.9) may now be solved for $\phi'(f)s$ using the integral representation of the solution (2.4). This gives

$$\phi'(f)s = -\int_{\Omega} G(f;\underline{x},\underline{x}')\, \nabla\cdot[s(\underline{x}')\nabla'\phi(f;\underline{x}')]\, dV' \tag{3.10}$$

$$= \int_{\Omega} \nabla' G(f;\underline{x},\underline{x}')\cdot\nabla'\phi(f;\underline{x}')\, s(\underline{x}')\, dV'$$

$$- \int_{\partial\Omega} G(f;\underline{x},\underline{x}')\, \frac{\partial}{\partial n'}\, \phi(f;\underline{x}')\, s(\underline{x}')\, dS' \tag{3.11}$$

from the generalization of Green's first theorem (2.3). The Green function $G(f;\underline{x},\underline{x}')$ satisfies

$$\nabla'\cdot[f(\underline{x}')\nabla' G(f;\underline{x},\underline{x}')] = \delta(\underline{x}-\underline{x}')$$

$$\text{and } G(\underline{x},\underline{x}') = 0 \quad \text{when } \underline{x}' \in \partial\Omega \ .$$

Thus the boundary integral term in (3.11) vanishes.

The update $s^{(k)}(\underline{x})$ in the Newton-Kantorovich method then satisfies the integro-differential equation

$$\int_{\Omega} G(f^{(k)};\underline{x},\underline{x}')\nabla'\cdot[s^{(k)}(\underline{x}')\nabla'\phi(f^{(k)};\underline{x}')]dV'$$

$$= \phi(f^{(k)};\underline{x})-\Phi(\underline{x}) \ , \ \underline{x} \in \Omega \tag{3.12}$$

or the integral equation

$$\int_{\Omega} \nabla' G(f^{(k)};\underline{x},\underline{x}')\cdot\nabla'\phi(f^{(k)};\underline{x}')s^{(k)}(\underline{x}')dV'$$

$$= \Phi(\underline{x})-\phi(f^{(k)};\underline{x}) \ , \ \underline{x} \in \Omega \ . \tag{3.13}$$

CASE 2

Neumann boundary conditions :

$$f\,\frac{\partial\phi(f)}{\partial n} = h \;,\; \underset{\sim}{x} \in \partial\Omega$$

and
$$\phi(f;\underset{\sim}{x}_0) = \phi_0 \;.$$

This gives

$$f\,\frac{\partial\phi'(f)s}{\partial n} + s\,\frac{\partial\phi(f)}{\partial n} = 0 \;,\; \underset{\sim}{x} \in \partial\Omega$$

or
$$f\,\frac{\partial\phi'(f)s}{\partial n} = -\,s\frac{\partial\phi(f)}{\partial n} \;,\; \underset{\sim}{x} \in \partial\Omega$$

and
$$\phi'(f)s\big|_{\underset{\sim}{x}=\underset{\sim}{x}_0} = 0 \;.$$

The equation (3.9) can now be solved using the integral representation of the solution (2.7). We obtain

$$\phi'(f)s = -\int_{\Omega} G(f;\underset{\sim}{x},\underset{\sim}{x}')\,\nabla'\cdot[s(\underset{\sim}{x}')\phi(f;\underset{\sim}{x}')]\,dV'$$
$$+\int_{\partial\Omega} G(f;\underset{\sim}{x},\underset{\sim}{x}')\,\frac{\partial}{\partial n'}\phi(f;\underset{\sim}{x}')s(\underset{\sim}{x}')\,dS' + c \;.$$

Here c is an arbitrary constant, and the modified Green function $G(f;\underset{\sim}{x},\underset{\sim}{x}')$ satisfies the conditions (2.6).

So

$$0 = \phi'(f)s\big|_{\underset{\sim}{x}=\underset{\sim}{x}_0} = -\int_{\Omega} G(f;\underset{\sim}{x}_0,\underset{\sim}{x}')\nabla'\cdot[s(\underset{\sim}{x}')\phi(f;\underset{\sim}{x}')]\,dV'$$
$$+\int_{\partial\Omega} G(f;\underset{\sim}{x}_0,\underset{\sim}{x}')\,\frac{\partial}{\partial n'}\phi(f;\underset{\sim}{x}')s(\underset{\sim}{x}')\,dS' + c$$

determining the constant c. Hence

$$\begin{aligned}\phi'(f)s = & -\int_{\Omega}[G(f;\underline{x},\underline{x}') - G(f;\underline{x}_0,\underline{x}')]\,\nabla'\cdot[s(\underline{x}')\phi(f;\underline{x}')]\,dV' \\ & +\int_{\partial\Omega}[G(f;\underline{x},\underline{x}') - G(f;\underline{x}_0,\underline{x}')]\,\frac{\partial}{\partial n'}\phi(f;\underline{x}')s(\underline{x}')\,dS' \\ & =\int_{\Omega}\nabla'[G(f;\underline{x},\underline{x}' - G(f;\underline{x}_0,\underline{x}')]\cdot\nabla'\phi(f;\underline{x}')s(\underline{x}')\,dV' \quad . \end{aligned} \tag{3.14}$$

The update $s^{(k)}(\underline{x})$ in the Newton-Kantorovich method then satisfies the integral equation

$$\int_{\Omega}\nabla'[G(f^{(k)};\underline{x},\underline{x}') - G(f^{(k)};\underline{x}_0,\underline{x}')]\cdot\nabla'\phi(f^{(k)};\underline{x}')s^{(k)}(\underline{x}')dV' = \Phi(\underline{x})-\phi(f^{(k)};\underline{x}), \quad \underline{x}\in\Omega\,. \tag{3.15}$$

Alternatively an integro-differential equation analogous to (3.12) is also satisfied.

In §3.5 at the end of this chapter we formally prove that the operator T is Fréchet differentiable in spaces of Hölder continuously differentiable functions - with Fréchet derivatives as have just been derived.

With both Dirichlet and Neumann boundary conditions we have obtained integral equations of the first kind to solve for the updates. For these integral equations (3.13) and (3.15) the existence, uniqueness and continuous dependence upon the measurements of their solutions may be established, under the same conditions as for the inverse problem as as whole in §3.1.

Suppose the measurement function satisfies the condition $\inf_{\Omega}|\nabla\Phi| > 0$, and there are Dirichlet boundary conditions on ϕ. Then from the discussion of the previous section, for a unique solution to the inverse problem, f must be known along the inflow boundary for example. Thus assuming the initial approximation, $f^{(0)}$ satisfies the specified values along the inflow boundary, then the constraint

$$s^{(k)} = 0 \text{ on the inflow boundary}$$

must be added to the equations (3.12) and (3.13). Then all subsequent iterates $f^{(k)}$ will have the correct values along the inflow boundary.

When there are Neumann boundary conditions on ϕ, and the measurement function $\Phi \in W^{2,\infty}(\Omega)$ and satisfies the condition (3.6), there is a unique solution to the inverse problem without the need to know f on the boundary. Then a constraint does not need to be added to the integral equation (3.15).

In §3.1 it was noted that the solution of the inverse problem depended continuously upon the first and second derivatives of the measurement function. This means the presence of noise in the measurements may produce large changes in the solution of the inverse problem. So if noise is present, we must use regularization techniques (see §1.4) when the integral equations of the first kind (3.13) and (3.15) are solved. Then physically realistic solutions would be obtained.

To solve the integral equations (3.13) and (3.15) measurements of ϕ are available only at discrete points of Ω corresponding to well sites. Then the right-hand side of the integral equations is known only at these discrete points. This requires the use of the collocation method to solve the integral equations. In this method the unknown function is expressed as a sum of basis functions

$$s^{(k)}(\underset{\sim}{x}) = \sum_{j=1}^{N} a_j g_j(\underset{\sim}{x}) \ . \tag{3.16}$$

The kernel and the right-hand side of the integral equation are then evaluated at the points where Φ is known. This gives us, for example, with the integral equation (3.13) arising from Dirichlet boundary conditions

$$\int_{\Omega} \left[\nabla' G(f^{(k)};\underline{x}_i,\underline{x}')\right] \cdot \nabla' \phi(f^{(k)};\underline{x}') \left[\sum_{j=1}^{N} a_j^{(k)} g_j(\underline{x}')\right] dV'$$
$$= \Phi(\underline{x}_i) - \phi(f^{(k)};\underline{x}_i) \text{ , } i \in \{1,...,M\} \text{ .}$$

Thus $\displaystyle\sum_{j=1}^{N} A_{ij}^{(k)} a_j^{(k)} = \Phi(\underline{x}_i) - \phi(f^{(k)};\underline{x}_i) \text{ , } i \in \{1,...,M\}$ (3.17)

where $\displaystyle A_{ij} = \int_{\Omega} \left[\nabla' G(f^{(k)};\underline{x}_i,\underline{x}')\right] \cdot \nabla' \phi(f^{(k)};\underline{x}') g_j(\underline{x}') \, dV'$ (3.18)

is the system of equations to be solved for $\underline{a}^{(k)}$. See §3.4 for numerical solutions of the integral equations that arise form a one-dimensional version of this inverse problem.

3.2.2 *Gauss–Newton Method*

In this subsection the Gauss-Newton method is derived for solving the system of nonlinear equations generated by a parameter identification approach to this inverse problem. The parameters to be determined are the coefficients in a basis function expansion for the unknown function f. That is

$$f(\underline{a};\underline{x}) = \sum_{j=1}^{N} a_j g_j(\underline{x}) \text{ .} \tag{3.19}$$

From the discussion on parameter identification in §1.5 the system of nonlinear equations to be solved for $\underline{a}$, and hence f is

$$r_i(\underline{a}) = \phi(\underline{a};\underline{x}_i) - \Phi(\underline{x}_i) = 0 \text{ , } i \in \{1,...,M\} \text{ .} \tag{3.20}$$

Here $\phi(\underline{a};\underline{x})$ is the solution of the direct problem, that is the p.d.e. (3.1) with coefficient function f given by (3.19) and either Dirichlet or Neumann boundary conditions. The measurements of ϕ are denoted by $\Phi(\underline{x}_i)$, $i \in \{1,...,M\}$. As was noted in §1.5 we require $M \geq N$.

As in the description of the Gauss-Newton method in §1.5 the Jacobian matrix of $\underline{r}(\underline{a})$ is required. From (3.20) the Jacobian elements for the system at the kth iteration are

$$J_{ij}^{(k)} = \frac{\partial r_i^{(k)}}{\partial a_j} = \frac{\partial}{\partial a_j}[\phi(\underline{a}^{(k)};\underline{x}_i] \ . \tag{3.21}$$

This means we require gradients of the function ϕ with respect to the unknown parameters. These gradients must be calculated from the direct problem formulation and its boundary conditions.

In addition to a local basis function expansion for f, Yeh and Yoon [1981] discretize the function ϕ in (3.1). They then take partial derivatives with respect to the unknown parameters giving systems of equations which the required gradients satisfy. We however will not discretize the problem any further at this stage, and will derive p.d.e's satisfied by the Jacobian elements.

Differentiation of

$$\nabla \cdot (f \nabla \phi) = \rho \ .$$

with respect to g_j gives

$$\nabla \cdot \left[\frac{\partial}{\partial a_j}(f \nabla \phi)\right] = 0 \ .$$

Thus

$$\nabla \cdot \left[f \nabla \frac{\partial \phi}{\partial a_j} + \frac{\partial f}{\partial a_j} \nabla \phi\right] = 0$$

and

$$\nabla \cdot \left[f^{(k)} \nabla \frac{\partial \phi^{(k)}}{\partial a_j}\right] = - \nabla \cdot (g_j \nabla \phi^{(k)}) \ , \ j \in \{1,...,N\} \tag{3.22}$$

from (3.19). Here $f^{(k)} = f(\underline{a}^{(k)};\underline{x})$ and $\phi^{(k)} = \phi(\underline{a}^{(k)};\underline{x})$.

This equation must be solved for the function $\frac{\partial \phi^{(k)}}{\partial a_j}(\underline{a}^{(k)};\underline{x})$. To do this boundary conditions for $\frac{\partial \phi}{\partial a_j}$ are required. Again there are two cases :

CASE 1 Dirichlet boundary conditions :

$$\phi(\underline{a};\underline{x}) = g(\underline{x}) \quad , \quad \underline{x} \in \partial\Omega \quad .$$

Thus
$$\frac{\partial \phi}{\partial a_j}(\underline{a};\underline{x}) = 0 \quad , \quad \underline{x} \in \partial\Omega \quad , \tag{3.23}$$

and so $\frac{\partial \phi}{\partial a_j}(\underline{a}^{(k)};\underline{x})$ satisfies homogeneous Dirichlet conditions.

CASE 2 Neumann boundary conditions :

$$f(\underline{x}) \frac{\partial \phi}{\partial n}(\underline{a};\underline{x}) = h(\underline{x}) \, , \, \underline{x} \in \partial\Omega$$

and
$$\phi(\underline{a};\underline{x}_0) = \phi_0$$

for some point $\underline{x}_0 \in \overline{\Omega}$.

Differentiation with respect to a_j gives

$$\frac{\partial f}{\partial a_j} \frac{\partial \phi}{\partial n}(\underline{a};\underline{x}) + f(\underline{x}) \frac{\partial}{\partial n}\left[\frac{\partial \phi}{\partial a_j}(\underline{a};\underline{x})\right] = 0 \quad .$$

Thus
$$f^{(k)}(\underline{x}) \frac{\partial}{\partial n}\left[\frac{\partial \phi}{\partial a_j}(\underline{a}^{(k)};\underline{x})\right] = - g_j(\underline{x}) \frac{\partial \phi}{\partial n}(\underline{a}^{(k)};\underline{x}) \tag{3.24}$$

and also
$$\frac{\partial \phi}{\partial a_j}(\underline{a}^{(k)};\underline{x}_0) = 0 \quad .$$

Therefore for both Dirichlet and Neumann conditions, in addition to the direct problem to be solved each iteration, N p.d.e's (3.22) must also be solved for the functions $\frac{\partial\phi^{(k)}}{\partial a_j}$, $j \in \{1,....,N\}$. These p.d.e's have the same coefficient function $f^{(k)}$ as the direct problem. The boundary conditions are of the same type as for the direct problem, being either the homogeneous Dirichlet conditions (3.23) or the Neumann conditions (3.24). The Jacobian elements (3.21) are then found from evaluating the functions $\frac{\partial\phi^{(k)}}{\partial a_j}$ at the points at which measurements of ϕ have been made.

Thus we have derived the Gauss-Newton method without resorting to any discretization in addition to the original formulation of the problem as a parameter identification problem. However, the use of numerical techniques such as the finite difference or finite element methods, will be necessary to solve both the direct problems and the p.d.e's for the Jacobian elements.

3.2.3 *Equivalence of Methods*

In this subsection we show that the discretized Newton-Kantorovich method (3.17) and the Gauss-Newton method produce the same sequence of approximate solutions. This is provided the same basis functions for f and the same measurements on ϕ are used in each case. This result is valid for general operator equations - see §1.5 - however it is instructive to prove the result in this special case.

Consider the case where there are Dirichlet boundary conditions on ϕ. Then an analytic expression may be obtained for the Jacobian elements from the p.d.e. (3.22). To do this note $\frac{\partial\phi^{(k)}}{\partial a_j}$ satisfies homogeneous Dirichlet conditions from (3.23) and then the integral representation for the solution (2.4) is used.

Hence

$$\frac{\partial r_i^{(k)}}{\partial a_j} = \frac{\partial \phi}{\partial a_j}(a^{(k)};\underline{x}_i) = - \int_\Omega G(f^{(k)};\underline{x}_i,\underline{x}')\nabla' \cdot [g_j(\underline{x}')\nabla' \phi(f;\underline{x}')] \, dV' \; . \tag{3.25}$$

From the formulation of the Gauss-Newton method (3.20) and (3.21)

$$\Sigma \frac{\partial r_i^{(k)}}{\partial a_j} s_j^{(k)} = \Phi(\underline{x}_i) - \phi^{(k)}(\underline{x}_i) \; , \; i \in \{1,...,M\} \tag{3.26}$$

is the system of equations to be solved for the update $\underline{s}^{(k)}$.

If however the generalization of Green's first theorem is used on (3.25), then we see this is the same system as (3.17) resulting from the discretization of the integral equation for the Newton-Kantorovich method. That is provided the basis functions used to solve the integral equation are the same as those used to discretize f in the Gauss-Newton method. Also measurements of ϕ obviously must be taken at the same points in each case.

Hence, under these conditions, the solution of the systems (3.17) and (3.26) is the same. Thus the update for the function f is the same with each method. It then follows that if the initial approximation is the same in each case, then so will be the resulting sequence of approximate solutions.

Essentially this means that linearizing the operator equation (3.8) and then discretizing it, produces the same results as first discretizing it and then linearizing. As was noted in §1.5, this result is true for general operator equations. However in practice we would not expect the two methods to produce exactly the same results. This is because the coefficients of the systems of equations (3.17) and (3.26) will be computed numerically in two different ways. The resulting errors in the coefficients will then most likely be different.

The advantage of the Newton-Kantorovich method is that no discretization of the inverse problem is necessary in its derivation. It then illustrates the nature of the linear operator equation to be solved at each iteration. However, for numerical implementation on this particular problem, the Gauss-Newton method we derived would generally be preferable. This is because the matrix elements of (3.26) are obtained directly from solving the N p.d.e.s (3.22). But to obtain the same matrix elements from discretizing the integral equation for the Newton-Kantorovich method is more complex. First M p.d.e.s must be solved to obtain the functions $G(\underline{x}_i,\underline{x}')$, $i \in \{1,...,M\}$. Moreover this Green function has a singularity at $\underline{x}=\underline{x}'$. Secondly, MxN integrals must be performed to obtain the matrix elements (3.17).

The advantages of indirect identification over direct identification for this inverse problem are also apparent. To implement both the Gauss-Newton method and the Newton-Kantorovich method we require only knowledge of the measurements Φ. This compares with direct identification where derivatives of Φ are required. In addition the points at which the measurements are known can be arbitrary points of Ω. However in the finite difference and finite element methods for direct identification, the measurement function or its derivatives are required at specified mesh points. Also when there is noise present in the measurements regularization techniques may be easily incorporated in the indirect identification approach. However direct identification, when it is feasible, is potentially simpler and less costly than indirect identification.

3.3 ONE-DIMENSIONAL PROBLEM

The one-dimensional form of the inverse problem considered in previous sections is

$$[f(x)\phi'(x)]' = \rho(x)\ , x\epsilon[a,b]\subset\mathbb{R}^1\ . \tag{3.27}$$

This differential equation can easily be integrated yielding

$$f(x) = \frac{1}{\phi'(x)}\left\{(f\phi')(P) + \int_P^x \rho(x')dx'\right\},\ x \in [a,b] \tag{3.28}$$

for some point $P \in [a,b]$. If $\phi'(x)$ is bounded away from zero over Ω and $f\phi'$ is given at P, then a unique solution exists for f. This inverse problem is clearly more stable than in higher dimensions. There f may vary as the second derivative of the measured function ϕ (see 3.4) rather than with the first derivative as above. However the problem is still unstable and regularization techniques must be used in the presence of measurement noise.

In the remainder of this section we examine the use of integral equation methods to solve a particular case of this one-dimensional problem. Some numerical results are presented - including the use of regularization.

3.3.1 *An Example*

Consider a problem where

$$[f(x)\phi'(x)]' = 0 \ ,$$

$$\phi(0) = 0 \ ,$$

$$\text{and} \qquad \phi(L) = V \ . \tag{3.29}$$

Figure 3.2 illustrates a two-dimensional situation which could arise in steady electric current or heat flow for example. This reduces to the one-dimensional problem (3.29).

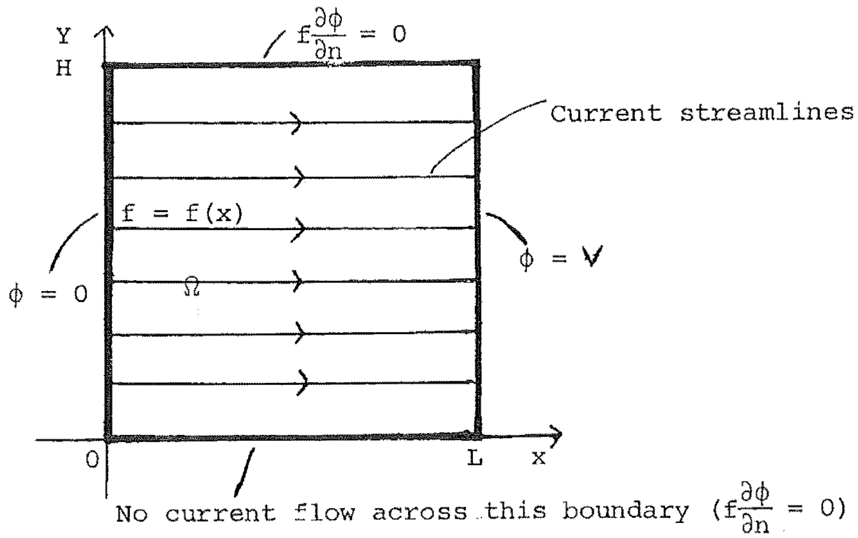

Figure 3.2

Solving (3.29) for f gives

$$f(x) = \frac{c}{\phi'(x)} \quad , \quad x \in [0,L] \quad . \tag{3.30}$$

Here c is a constant which must be determined from some additional information. This is similar to the two-dimensional Dirichlet problem of the previous sections where extra knowledge of the function f was required to give a unique solution to the inverse problem.

Consider solving for the resistivity h = 1/f instead of the conductivity f. From (3.30)

$$\begin{aligned} \phi(x) &= c \int_0^x \frac{dx'}{f(x')} \\ &= c \int_0^x h(x')dx' \quad . \end{aligned} \tag{3.31}$$

Then

$$V = \phi(L) = c \int_0^L h(x')dx'$$

and

$$c = \frac{V}{\int_0^L h(x')dx'}$$

$$= \frac{VL}{\bar{h}} \quad . \tag{3.32}$$

Here

$$\bar{h} = \frac{1}{L} \int_0^L h(x')dx'$$

is the mean value of h(x) over [0,L].

This gives from (3.30)

$$h(x) = \frac{\bar{h}}{VL}\phi'(x) \quad , \quad \underset{\sim}{x} \in [0,L] \ . \tag{3.33}$$

Henceforth we assume knowledge of $\bar{h}$ as our additional information to uniquely determine the function h(x). There is then a linear relationship between h(x) and $\phi(x)$ the function of which measurements are to be made.

3.3.2 *An Integral Equation*

Assume we are given an initial approximation $h^{(0)}(x)$ to the resistivity. This approximation is required to have the given mean value, that is

$$\frac{1}{L}\int_0^L h^{(0)}(x')dx' = \bar{h}$$

If the methods of the previous section are used the following integro-differential equation is obtained for $s^{(0)}(x) = h^{(1)}(x) - h^{(0)}(x)$, the update in the Newton-Kantorovich method

$$\int_0^L G(h^{(0)};x,x')\left[\frac{\phi'(h^{(0)};x')s^{(0)}(x)}{[h^{(0)}(x')]^2}\right]'dx' = \Phi(x)-\phi(h^{(0)};x) \ , \ x \in [0,L] \tag{3.34}$$

subject to the constraint

$$\int_0^L s^{(0)}(x')dx' = 0 \ .$$

Here $G(h^{(0)};x,x')$ is the Green function for the Dirichlet problem (3.29), and

$\phi(h^{(0)};x)$ the solution of this problem with coefficient $h^{(0)}(x)$. $\Phi(x)$ denotes the measurements that are made of $\phi(h;x)$. However since this problem is linear, solving this equation gives the exact solution $h(x) = h^{(1)}(x)$. Integration by parts gives the integral equation

$$\int_0^L \frac{\partial}{\partial x'} G(h^{(0)};x,x') \frac{\phi'(h^{(0)};x')}{[h^{(0)}(x')]^2} s^{(0)}(x')dx' = \phi(h^{(0)};x) - \Phi(x)$$

$$\text{s.t.} \quad \int_0^L s^{(0)}(x')dx' = 0 \ . \tag{3.35}$$

It should be noted that $s^{(0)}(x) = h^{(0)}(x)$ satisfies the homogeneous form of the integro-differential equation (3.34) - without the constraint. The function $h^{(0)}(x)$ is then also a solution of the homogeneous integral equation and so this equation is singular in nature. It follows that to any solution of the integral equation any arbitrary multiple of $h^{(0)}(x)$ may be added. However, when the constraint is imposed, a unique solution is obtained.

If we choose $h^{(0)}(x) = \hbar$, a constant initial approximation, then $\phi(h^{(0)};x)$ and $G(h^{(0)};x,x')$ may be determined analytically. From (3.29) if $L = 1$ then

$$\phi(\hbar;x) = Vx \ . \tag{3.36}$$

Also

$$G(\hbar;x,x') = \begin{cases} \hbar(x-1)x' \ , & 0 \leq x' \leq x \\ \hbar x(x'-1) \ , & x < x' \leq 1 \end{cases}$$

giving

$$\frac{\partial G}{\partial x'}(\hbar;x,x') = \begin{cases} \hbar(-1) \ , & 0 \leq x' \leq x \\ \hbar x \ , & x < x' \leq 1 \ . \end{cases} \tag{3.37}$$

In the next subsection numerical results from solving the resulting integral equation are presented.

To solve this inverse problem we have chosen to use integral equation methods rather than use the explicit form of the solution (3.33). This is because in the presence of measurement noise the measured function $\Phi(x)$ will generally not be differentiable. A solution does not then exist in the classical sense. However solving an integral equation allows us to incorporate regularization methods and so obtain a "solution".

The integral equation given by (3.31) could also be solved for h(x). However we prefer to solve the singular integral equation (3.35) with constraint, as this is similar to the equation that arises from the Dirichlet problem in higher dimensions.

3.4 NUMERICAL IMPLEMENTATION

This section contains some numerical results from the solution of the one-dimensional inverse problem of the previous section. Reconstruction in the presence of measurement noise are presented as well as solutions when the data is exact.

The integral equation to be solved is (3.35). With a constant initial approximation from (3.36) and (3.37) this becomes

$$\frac{V}{\hbar}\int_0^L K(x,x')\, s(x')\, dx' = Vx - \Phi(x)$$

$$\text{s.t.} \quad \int_0^L s(x')\, dx' = 0 \, , \tag{3.38}$$

where $$K(x,x') = \begin{cases} x-1 \, , & 0 \le x' \le x \\ x \, , & x \le x' \le 1 \, . \end{cases}$$

To solve this integral equation the collocation method was used. The basis functions utilized were piecewise constant functions and linear or quadratic B-splines. The integrals were performed numerically with an adaptive integration package.

The number of measurements used for the reconstructions exceeded the number of basis functions. This gave an overdetermined system of linear equations. These were solved by the least squares method and singular value decomposition (S.V.D.) techniques (Golub and Kahan [1965]).

All numerical computations were performed on a PRIME P750 digital computer in single precision. With this precision the machine epsilon, denoted by ϵ and which is defined as the smallest number such that $1 + \epsilon > 1$, is approximately 10^{-7}. All integrals were evaluated with an adaptive Simpson's rule to a relative accuracy of 10^{-6}.

3.4.1 *S.V.D. Regularization*

The regularization method used when measurement noise was present was also based upon singular value decomposition methods. This method scales the singular values, s_j, by a filter factor

$$\frac{s_j^{\,r}}{s_j^{\,r} + \alpha^r} .$$

This factor is close to one for $s_j > \alpha$ and tends to zero as $s_j \rightarrow 0$. Thus the effect of the smaller singular values which cause ill-conditioning is eliminated. The larger we choose α the smoother the solution is but the more information that is lost. The exponent r determines the roll-off of the filter. As $r \rightarrow \infty$ a square filter is obtained with singular values $s_j < \alpha$ chopped out, whereas if $r = 1$ or 2 a smoother roll-off is obtained.

The relationship between S.V.D. and Tikhonov regularization is given in Betero *et al.* [1979]. See also Hansen [1971], O'Brien and Wall [1980] and Wall [1980] for more detailed descriptions of the use of S.V.D. techniques for solving first kind integral equations.

3.4.2 *Numerical Results*

A variety of different functions were reconstructed.

(i) Straight line : $h(x) = 1 + x \;, x \in [0,1]$.

We utilized 10 basis partitions. The basis functions used were piecewise constant functions with 10 test points and linear B-splines with 20 test points. The condition numbers of the matrices obtained were 40 and 17 respectively. The resulting reconstructions are plotted in Figure 3.3. There was negligible error in the solution when linear B-splines were used as a straight line can be represented exactly by these functions. Also it should be noted we have exact data here, i.e. no measurement noise. Reconstructions of a straight line in the presence of measurement noise are outlined in (iv). The solution was also well approximated by piecewise constant functions as can be seen from Figure 3.3.

(ii) Step function : $h(x) = \begin{cases} 1\,, & 0 \le x \le \frac{1}{2} \\ 2\,, & \frac{1}{2} < x \le 1 \end{cases}$.

Piecewise constant basis functions were used with 10 basis partitions and 15 test points. The condition number of the matrix obtained was 9.8. The resulting reconstruction is plotted in Figure 3.4. Again there was negligible error in the solution as a step function may be represented exactly by piecewise constant functions when the discontinuity coincides with a point of partition.

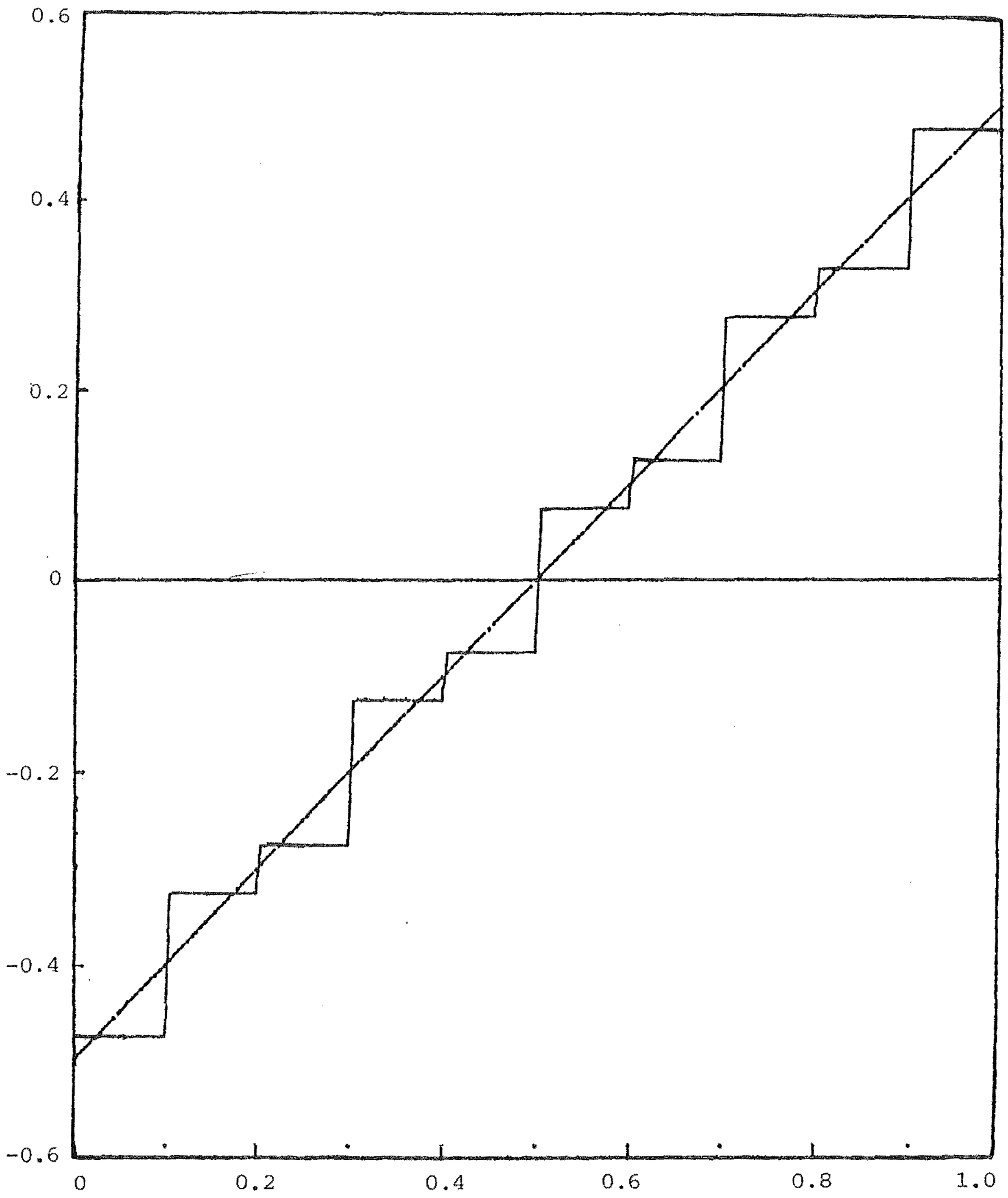

Figure 3.3

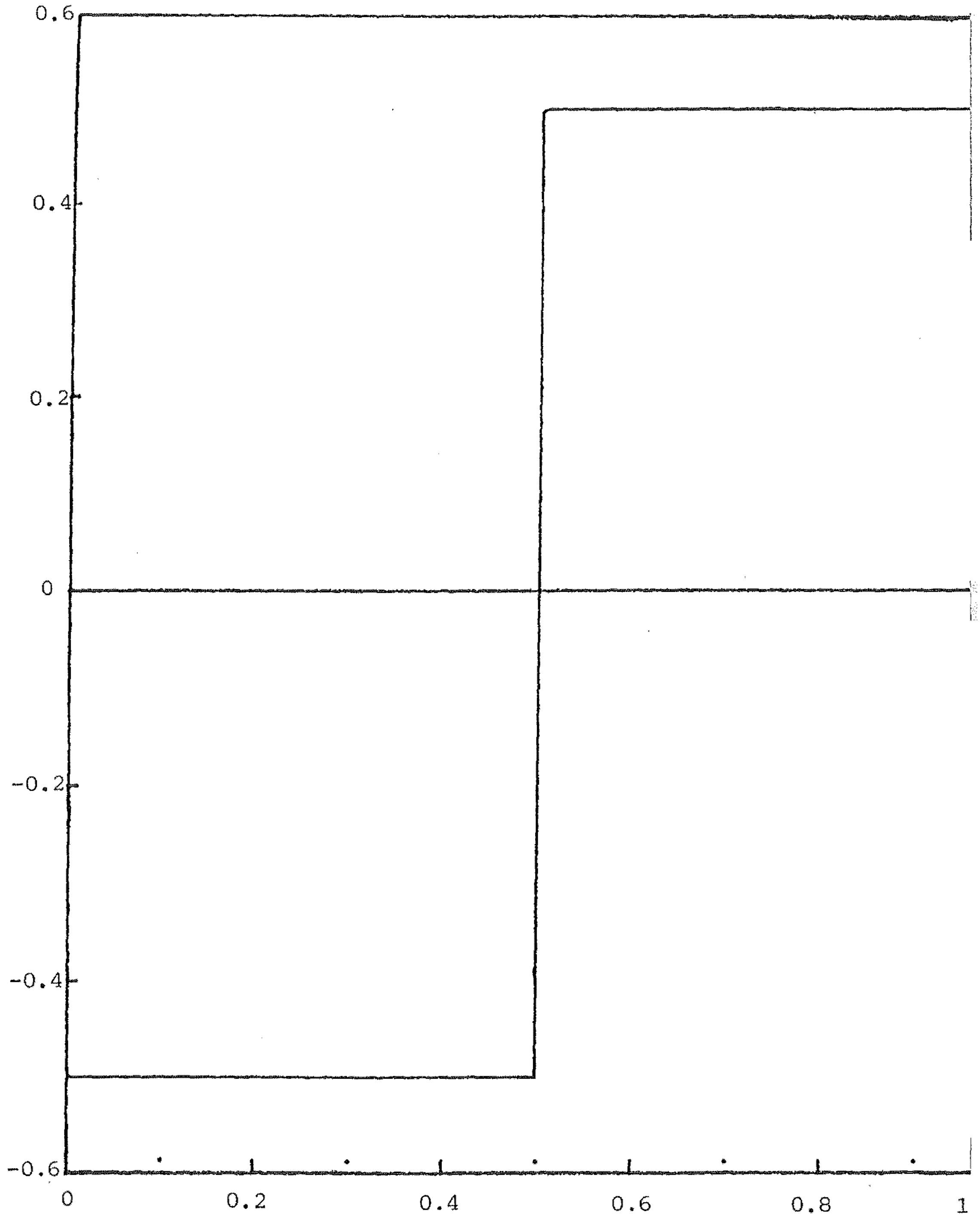

Figure 3.4

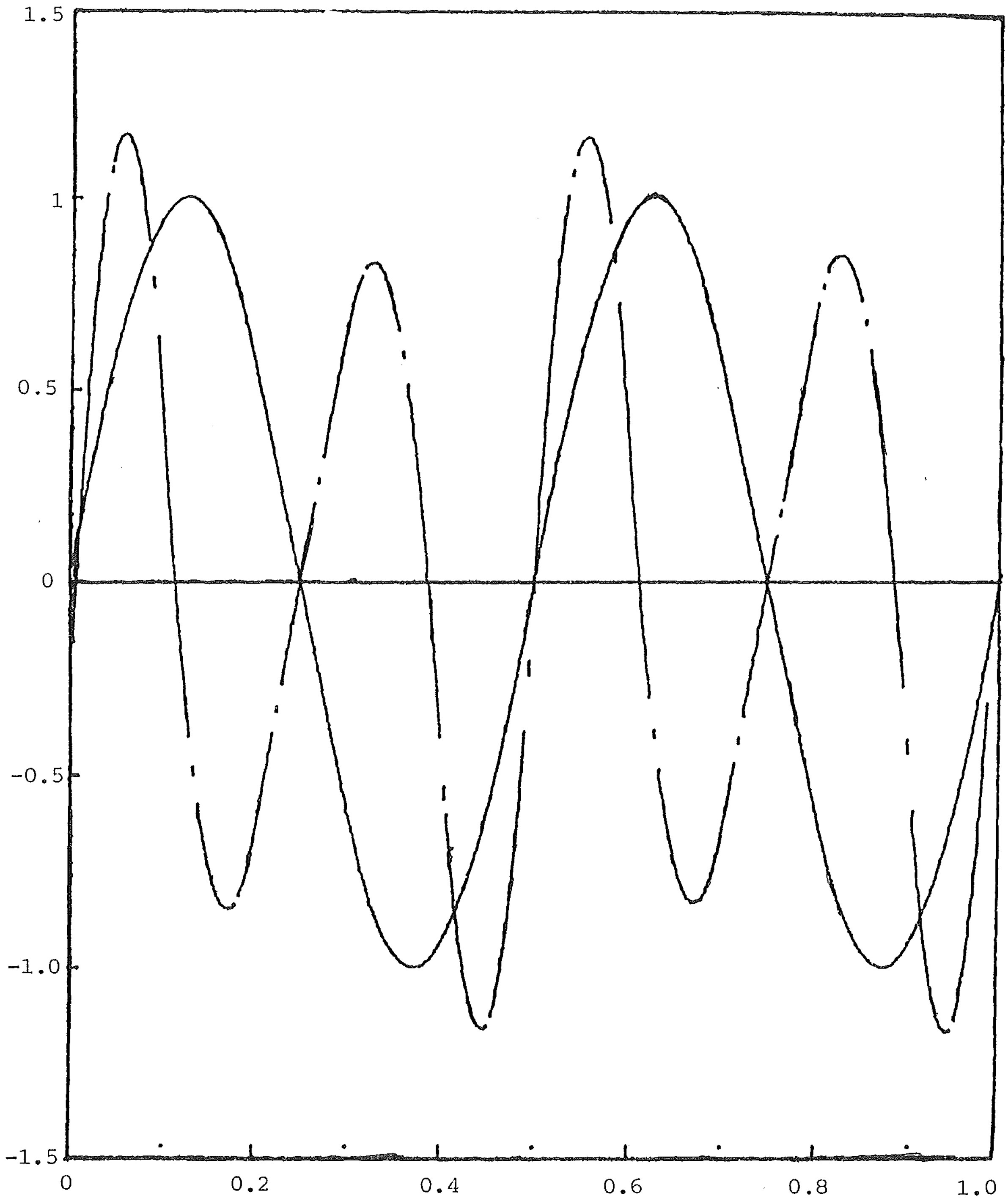

Figure 3.5

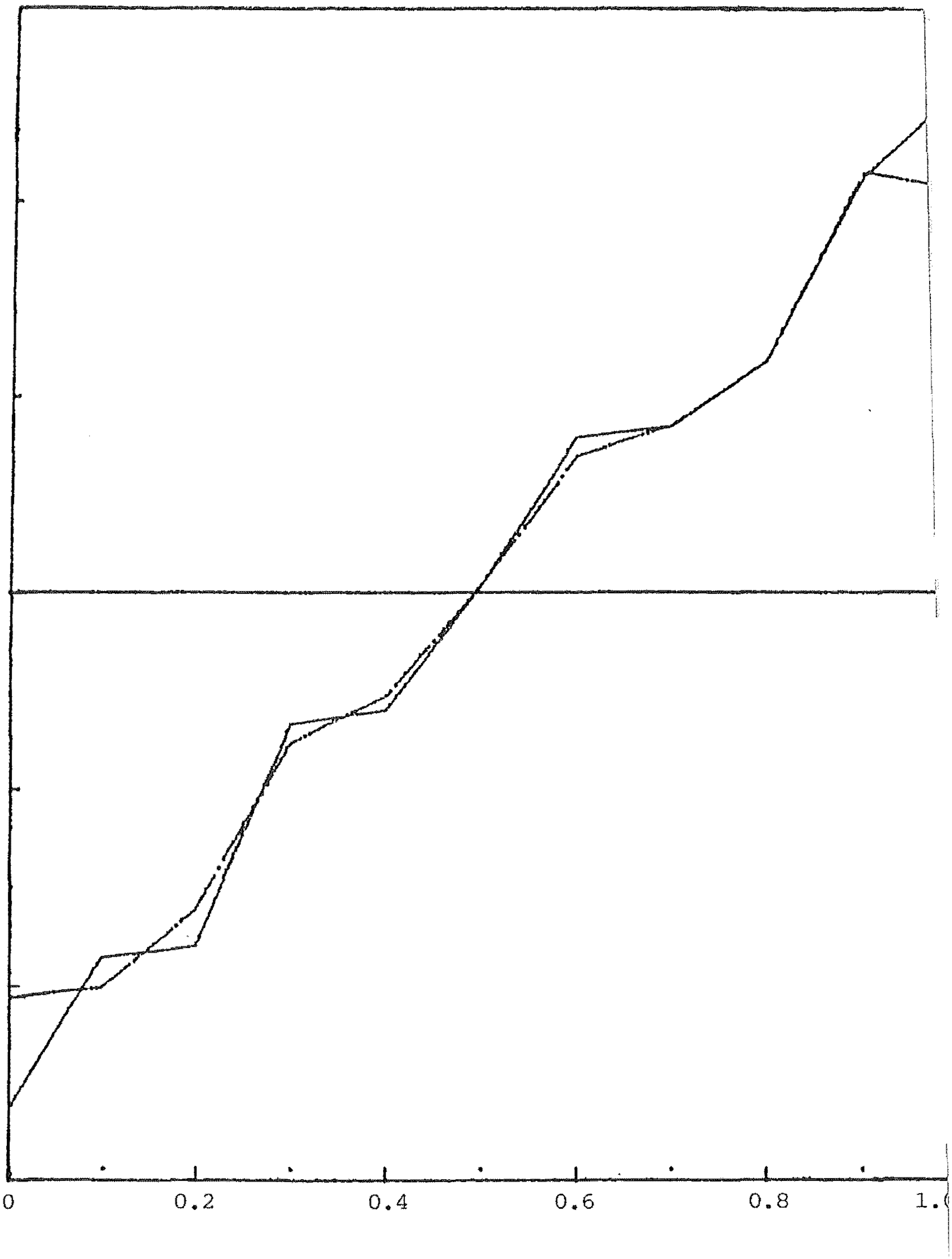

Figure 3.6 ($\frac{1}{2}$% noise)

(a) Unregularized Solution ————

(b) Regularized Solution —·—·—·

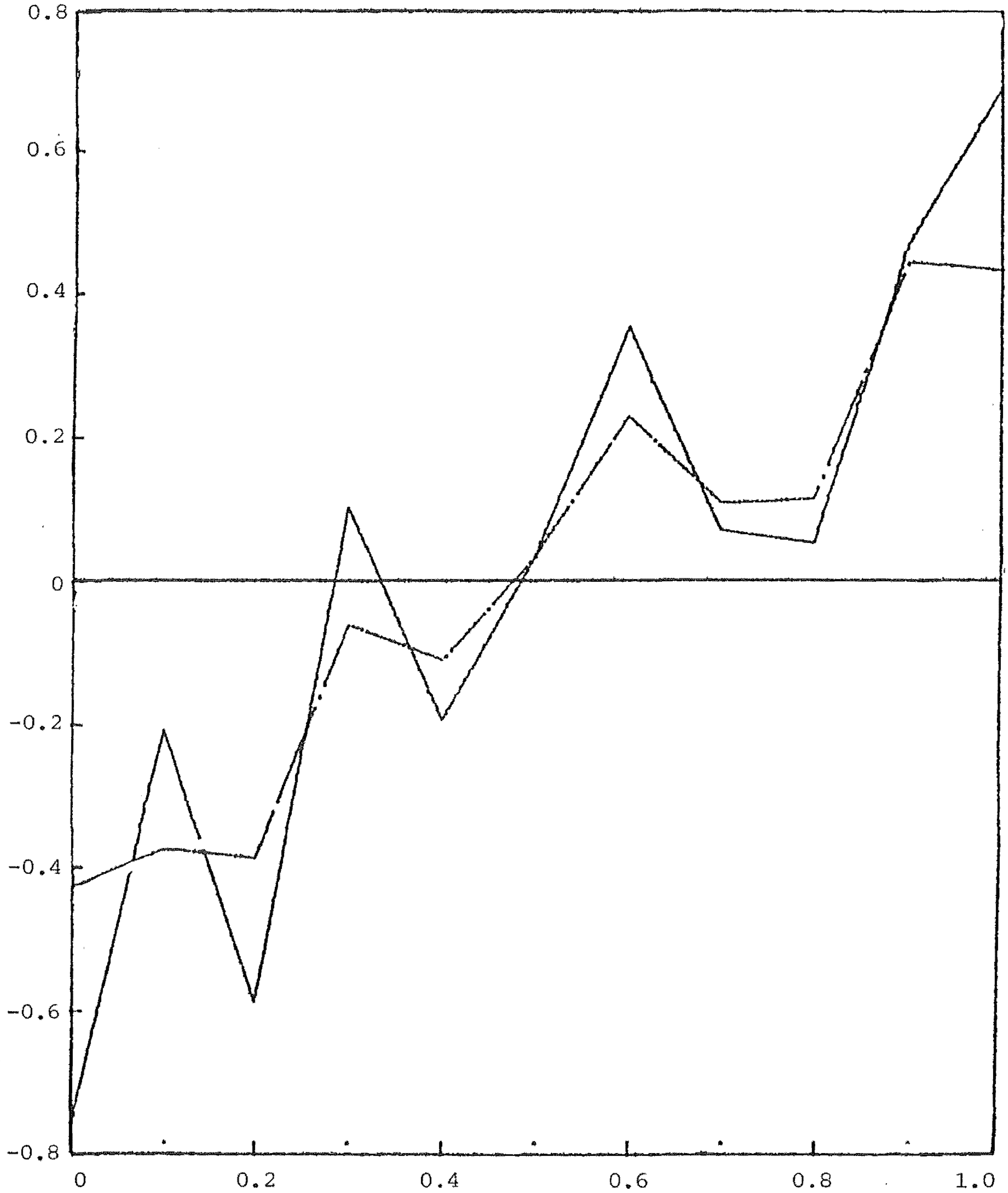

Figure 3.7 (2% noise)

(a) Unregularized Solution

(b) Regularized Solution

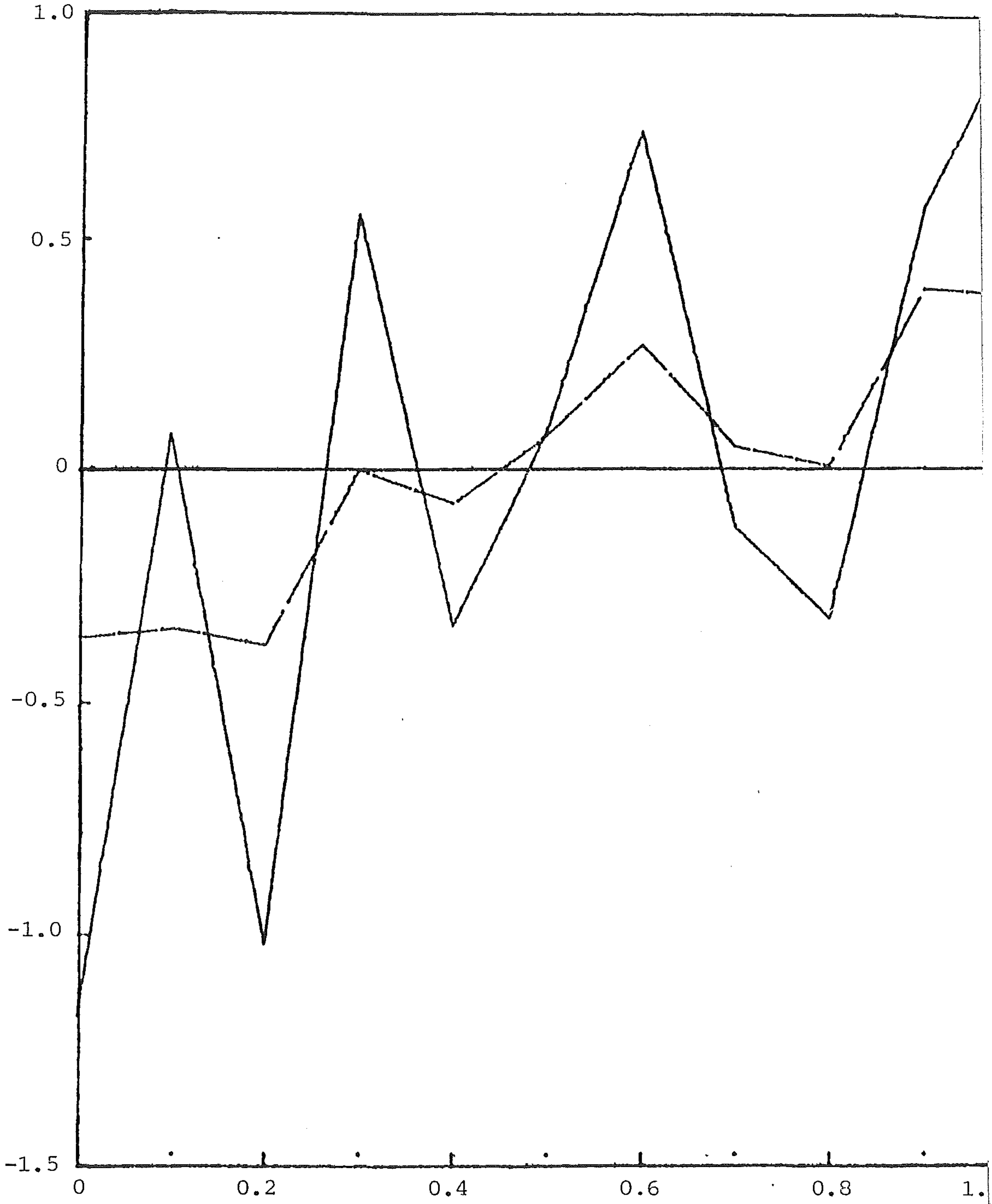

Figure 3.8 (5% noise)

(a) Regularized Solution

(b) Unregularized Solution

(iii) Trigonometric function : $h(x) = 1.5 + \sin(2\pi\omega x)$, $\omega = 2,4$.

Quadratic B-splines were utilized, again with 10 basis partitions and 15 test points. The solution was approximated well in the ω=2 case, as can be seen from Figure 3.5. When ω=4 the solution, as would be expected, is not quite as accurate - however it is still reasonable.

(iv) Straight line with measurement noise.

As in (i) $h(x) = 1 + x$ with linear B-splines for basis functions. The noise we used was uniformly distributed. The S.V.D. regularization method previously described was utilized. We set $r = 1$ as it was found this gave better results than $r = 2$ or greater, when the size of the update was reduced rather than smoothing taking place.

The updates with $\frac{1}{2}$% noise is plotted in Figure 3.6. For each case we plot both the update with and without regularization. With $\alpha = 0.065$ some smoothing of the solution takes place in the middle of the interval, however at the end points there is a marked degradation of the solution.

With 2% noise the unregularized solution becomes more oscillatory and the smoothing effect of the regularization, with $\alpha = 0.12$, becomes more apparent. At the 5% noise level the unregularized solution "blows up" and becomes highly oscillatory. The need for regularization is then clear. Here we set $\alpha = 0.35$. Note the optimum value of α increases with the increase in noise - which is to be expected as more smoothing is required.

In summary with this integral equation approach the solution of the inverse problem is well approximated - even in the cases of discontinuous and oscillatory functions. In addition, physically realistic solutions may be obtained in the presence of measurement noise using regularization methods.

It should be noted that although this inverse problem is one-dimensional and linear, we could expect similar behaviour from integral equation solutions fo[r] the nonlinear problem in higher dimensions. However, as the solution the[n] depends on the second rather than first derivatives of the measurement function some increase in instability in the presence of measurement noise would be expected.

Due to the relatively low condition numbers of the matrices obtained (as the singular values decayed only slowly) this problem (and its two and three dimensional counterparts) would be classified as mildly ill-posed. This compares with the boundary measurement version of the inverse problem (outlined in §3.6) where the singular values are exponentially decreasing, asymptotically (see the Appendix). That problem would be classified as severely ill-posed.

3.5 THEORETICAL CONSIDERATIONS

In this section we examine several theoretical aspects of the operator equation. First Fréchet differentiability of the operator with classical solutions is proven. This implies continuity of the map. It is then shown that it is in fact Lipshitz continuous if the solution is restricted to lie in a bounded set. Then some questions connected with stability are considered. The Fréchet derivative is shown to be a compact operator. The problem is then reformulated as a minimization over a compact set, and the existence of a solution to such a problem is proven.

3.5.1 *Fréchet Differentiability*

In this section it is formally shown that within the classical regularity theory the field, ϕ, depends continuously upon the coefficient function, f. Moreover, this map is Fréchet differentiable with Fréchet derivative as derived earlier. The Dirichlet problem only is considered. However results may be proved for the

Neumann problem in a similar manner.

Spaces of Hölder continuously differentiable functions are utilized. The direct problem is

$$\nabla \cdot (f \nabla \phi) = \rho \ , \ \underset{\sim}{x} \in \Omega$$
$$\phi = g \ , \ \underset{\sim}{x} \in \partial\Omega \ . \tag{3.39}$$

The domain Ω is required to be convex and smooth ($C^{2,\alpha}$). In addition $\rho \in C^{0,\alpha}(\overline{\Omega})$ and $g \in C^{2,\alpha}(\partial\Omega)$. Consider f belonging to the open set $X_0 = \{f: f \in C^{1,\alpha}(\Omega) \ , \ f > 0\}$. From Chapter 2 we have :

LEMMA 3.1

For $f \in X_0$ there exists a unique solution $\phi \in C^{2,\alpha}(\overline{\Omega})$ of (3.39). Moreover, when $g = 0$

$$\|\phi\|_{2,\alpha} \leq K\|\rho\|_{0,\alpha} \ . \qquad \square$$

Henceforth we denote by $\phi(f;\underset{\sim}{x})$ or just $\phi(f)$ the solution of the direct problem for a given f.

THEOREM 3.1

The map $f \rightarrow \phi(f)$ from $X_0 \rightarrow C^{2,\alpha}(\overline{\Omega})$ is Fréchet differentiable with

$$\phi'(f)s(\underset{\sim}{x}) = - \int_{\Omega} G(f;\underset{\sim}{x},\underset{\sim}{x}') \ \nabla' \cdot [s(\underset{\sim}{x}')\nabla' \phi(f;\underset{\sim}{x}')] \ dV' \ . \tag{3.40}$$

<u>Proof</u> To apply the implicit function theorem (THEOREM 1.1) ϕ must belong to a linear space. The function $g \in C^{2,\alpha}(\partial\Omega)$ may be extended to some function $\tilde{\phi} \in C^{2,\alpha}(\overline{\Omega})$ - see Gilbarg and Trudinger [1983] p.92.

Then $\overline{\phi} = \phi - \tilde{\phi}$ satisfies

$$\nabla\cdot(f\nabla\overline{\phi}) = \rho - \nabla\cdot(f\nabla\tilde{\phi}) = \tilde{\rho} \ , \ \underline{x} \in \Omega$$
$$\overline{\phi} = 0 \ , \ \underline{x} \in \partial\Omega \ .$$

Noting that $\phi'(f)s = \overline{\phi}'(f)s$ we need only consider the homogeneous problem requiring the solution to belong to $Y_0 = \{\phi \in C^{2,\alpha}(\overline{\Omega}) \ , \ \phi = 0 \text{ on } \partial\Omega\}$.

Set $\xi(f,\phi) = \nabla\cdot(f\nabla\phi) - \rho$, then $\xi : X_0 \otimes Y_0 \rightarrow C^{0,\alpha}(\overline{\Omega})$.

We now check the conditions of the implicit function theorem.

1. We have
$$\begin{aligned} &||\xi(f+\delta f, \ \phi+\delta\phi) - \xi(f,\phi)||_{0,\alpha} \\ &= ||\nabla\cdot(f\nabla\delta\phi) + \nabla\cdot(\delta f\nabla\phi) + \nabla\cdot(\delta f\nabla\delta\phi)||_{0,\alpha} \\ &\leq \gamma(||f||_{1,\alpha}||\delta\phi||_{2,\alpha} + ||\delta f||_{1,\alpha}||\phi||_{2,\alpha} + ||\delta f||_{1,\alpha}||\delta\phi||_{2,\alpha}) \ . \end{aligned}$$

Here the result $||\nabla\cdot(f\nabla\phi)||_{0,\alpha} \leq \gamma||f||_{1,\alpha}||\phi||_{2,\alpha}$ has been used.

Thus $\xi(f,\phi)$ is continuous.

2. The partial Fréchet derivative of ξ with respect to f is

$$\xi_f(f,\phi)s = \nabla\cdot(s\nabla\phi) \ .$$

Therefore

$$\begin{aligned} &||\xi_f(f+\delta f, \ \phi+\delta\phi)s - \xi_f(f,\phi)s||_{0,\alpha} \\ &= ||\nabla\cdot(s\nabla\delta\phi)||_{0,\alpha} \\ &\leq \gamma||\phi||_{2,\alpha} \ ||s||_{1,\alpha} \ . \end{aligned}$$

Thus $\xi_f(f,\phi)$ is continuous in f and ϕ.

The partial Fréchet derivative of ξ with respect to ϕ is $\xi_\phi(f,\phi)t = \nabla\cdot(f\nabla t)$, and so $\xi_\phi(f,\phi)$ may be shown to be continuous in f and ϕ in a similar manner to ξ_f.

3. $[\xi_\phi(f,\phi)]^{-1}$ is bounded from Lemma 3.1.

Hence from the implicit function theorem (THEOREM 1.1)

$$\phi'(f)s = -[\xi_\phi(f,\phi)]^{-1}\xi_f(f,\phi)s \quad .$$

Now $[\xi_\phi(f,\phi)]^{-1}u = \int_\Omega G(f;\underline{x},\underline{x}')\, u(\underline{x}')\, dV'$ and the desired result follows.

□

So our operator is Fréchet differentiable, moreover the expression for the Fréchet derivative we derived in a fairly intuitive manner is correct.

Thus we have Fréchet differentiability of the operator for classical solutions of the direct problem. We note Chavent [1973] has proved the analogous result for weak solutions i.e. from $\{f \in L^\infty(\Omega), f > 0\}$ into $H^1(\Omega)$. The result is also for Dirichlet boundary conditions and the implicit function theorem is utilized. However in this case an explicit formula such as (3.40) for the Fréchet derivative was not obtained.

The two results - ours and Chavent's are complimentary. Chavent's obviously needs weaker assumptions on the function to be reconstructed (continuity and differentiability of the coefficient function are not required). However ours has a stronger function space for the range - $C^{1,\alpha}$ rather than H^1. For example, our result allows for point measurements whereas Chavent's does not in $\mathbb{R}^2$ or $\mathbb{R}^3$.

The Fréchet differentiability of the operator implies that it is continuous. We now examine what additional assumptions are necessary in order to show that it is either bounded or Lipschitz continuous.

3.5.2 *Lipschitz Continuity*

In order to obtain boundedness (see §1.5.5) of our operator, f is required to belong to the following subset of $C^{1,\alpha}$:

$$X_1 = \{f \in C^{1,\alpha}(\overline{\Omega}) \ , \ f \geq c > 0\} \ .$$

To obtain Lipschitz continuity (see §1.5.4) of the map, f must belong to the bounded subset of $C^{1,\alpha}$:

$$X_2 = \{f \in C^{1,\alpha}(\overline{\Omega}) \ , \ \|f\|_{1,\alpha} \leq M \ , \ f \geq c > 0\} \ .$$

THEOREM 3.2

The map $f \rightarrow \phi(f)$ from

(i) $X_1 \rightarrow C^{2,\alpha}(\overline{\Omega})$ is bounded,

(ii) $X_2 \rightarrow C^{2,\alpha}(\overline{\Omega})$ is Lipschitz continuous .

<u>Proof</u> (i) We must show that bounded sets of X_1 are mapped to bounded sets $C^{2,\alpha}$ i.e. if $f \in X_1$ and $\|f\|_{1,\alpha} \leq M_0$ then $\|\phi(f)\|_{2,\alpha} \leq N_0$, for some N_0.

Now from THEOREM 2.1

$$\|\phi(f)\|_{2,\alpha} \leq K(\|\rho\|_{0,\alpha} + \|g\|_{2,\alpha}) \ .$$

K depends only upon α, c, M_0 and the diameter of Ω (see Courant and Hilbert [1962], p.335) giving the desired result.

(ii) To prove this result we must show

$$||\phi(f+\delta f) - \phi(f)||_{2,\alpha} \leq \xi||\delta f||_{1,\alpha}$$

where ξ is independent of f, that is depends only upon α, c, M ; the source term ρ, the boundary data g, and the region Ω.

Now

$$\nabla\cdot[f\nabla\phi(f)] = \rho \ , \ \ \phi(f) = g \text{ on } \partial\Omega$$

and

$$\nabla\cdot[(f+\delta f)\nabla\phi(f+\delta f) = \rho \ , \ \ \phi(f+\delta f) = g \text{ on } \partial\Omega \ .$$

Subtracting gives

$$\nabla\cdot\{(f+\delta f)\nabla[\phi(f+\delta f) - \phi(f)]\} = -\nabla\cdot[\delta f\nabla\phi(f)]$$

and

$$\phi(f+\delta f) - \phi(f) = 0 \ \text{ on } \ \partial\Omega.$$

LEMMA 3.1 gives

$$||\phi(f+\delta f) - \phi(f)||_{2,\alpha} \leq K||\nabla\cdot[\delta f\nabla\phi(f)]||_{0,\alpha} \ .$$

K depends only upon α,c,M and the diameter of Ω.

Using the result $||\nabla\cdot(f\nabla\phi)||_{0,\alpha} \leq \gamma||f||_{1,\alpha}||\phi||_{2,\alpha}$ gives

$$||\phi(f+\delta f) - \phi(f)||_{2,\alpha} \leq K\gamma||\phi(f)||_{2,\alpha}||\delta f||_{1,\alpha} \ .$$

From THEOREM 2.1

$$||\phi(f)||_{2,\alpha} \leq K(||\rho||_{0,\alpha} + ||g||_{2,\alpha}) \ .$$

So that

$$||\phi(f+\delta f) - \phi(f)||_{2,\alpha} \leq \xi||\delta f||_{1,\alpha} \ ,$$

where $$\xi = K^2\gamma(\|p\|_{0,\alpha} + \|g\|_{2,\alpha})$$

is independent of f as required. □

The direct method of proof in THEOREM 3.2 did not require the use of the implicit function theorem in contrast to that for continuity/Fréchet differentiability in THEOREM 3.1. We note (ii) could also have been arrived at via the mean value theorem for operators THEOREM 1.2 and the Fréchet differentiability result with

$$\xi = \sup_{f \in X_1} \|\phi'(f)\| \ .$$

The Lipschitz continuity result (THEOREM 3.2 (ii)) gives a bound on the change in the direct problem solution, ϕ, that results from a change in the coefficient, f. This is complimentary to a result from Richter [1986a] applicable to weak solutions - see also the Appendix.

So in summary the map $f \rightarrow \phi(f)$ into $C^{2,\alpha}(\overline{\Omega})$ is continuous (and Fréchet differentiable) for $f \in C^{1,\alpha}(\overline{\Omega})$ and $f > 0$. To obtain boundedness of the map the constraint $f \geq c > 0$ must be imposed on the domain. Finally to obtain Lipschitz continuity, f must also belong to the bounded subset, $\|f\|_{1,\alpha} \leq M$.

3.5.3 *Compactness*

In this subsection we use the result for the boundedness of $\phi(f)$ just derived to prove compactness of T(f). The approach suggested in §1.5.5 is used, with the measurements belonging to a suitably chosen function space.

In the following theorem, Z may be either $L^2(\Omega)$ or $C^0(\Omega)$.

THEOREM 3.3

The operators $T(f) : X_1 \rightarrow Z$ and $T'(f) : C^{1,\alpha}(\overline{\Omega}) \rightarrow Z$ with $f \in X_0$, are compact.

Proof The operators $T(f) : X_1 \to C^{2,\alpha}(\overline{\Omega})$ and $T'(f) : C^{1,\alpha}(\overline{\Omega}) \to C^{2,\alpha}(\overline{\Omega})$ are bounded from THEOREMS 3.2 and 3.1 respectively. As the imbedding $C^{2,\alpha}(\overline{\Omega}) \to Z$ is compact, the result follows as the composition of a compact operator and a bounded operator is compact from THEOREM 1.3 (i). □

The inverse of a compact operator is unbounded - see THEOREM 1.3 (ii). The solution of the fully nonlinear inverse problem (or its linearization) is then on an ill-posed problem, with Z specified as above. In particular the inverse problem will be unstable for point measurements of ϕ (from setting $Z = C^0(\overline{\Omega})$) or distributed measurements with $Z = L^2(\Omega)$.

We note also that as Chavent proved Fréchet differentiability for weak solutions from $\{f \epsilon L^{\infty}(\Omega) \ , \ f > 0\}$ into $H^1(\Omega)$, it follows for such solutions the Fréchet derivative of the map is also compact into $L^2(\Omega)$. We expected such a result as from §3.1 the solution of the inverse problem (in the L^{∞} norm) depends upon the second derivatives of the measured potential.

So in order to guarantee the existence of a solution to the inverse problem, in the next subsection we apply regularization techniques to the problem. However no actual results for the regularized problem are proven.

3.5.4 *Regularization*

In the last section we presented some numerical results from the use of the S.V.D. regularization method. However with that approach it is difficult to prove theoretical results, so the application of the Tikhonov selection method (outlined in §1.3.2) is investigated.

Consider point measurements of ϕ at $\{\underline{x}_i\}$, $i = \{1, \dots ,M\}$. The operator equation to be solved is

$$T(f) = \phi(f;\underline{x}_i) - \Phi(\underline{x}_i) = 0 \ , \ i \epsilon \{1, \dots ,M\} \ . \tag{3.41}$$

From THEOREM 3.3 this operator is compact. Its solution is therefore unstable and may not even exist. We shall make use of the classical regularity theory from Courant and Hilbert and the Fréchet differentiability result just derived.

To regularize the inverse problem the solution is restricted to lie within a suitable compact set - see §1.5.5. Consider the following problem

$$\text{minimize} \qquad ||T(f)||^2 = \sum_{i=1}^{M} [\phi(f;\underline{x}_i) - \Phi(\underline{x}_i)]^2 \tag{3.42}$$

subject to $f \in X_2$, where X_2 is a compact subset of $C^{1,\alpha}(\overline{\Omega})$.

One possible choice for X_2 is

$$X_2 = \{f \in C^{1,\alpha}(\overline{\Omega}) : ||f||_{1,\beta} \leq M \ , \ f \geq c > 0\} \ .$$

The constants β (with $\beta > \alpha$), c and M are given *a priori*, and the compactness of the imbedding follows from the compactness of the imbedding $C^{1,\beta}(\overline{\Omega}) \rightarrow C^{1,\alpha}(\Omega)$, with $\beta > \alpha$ (Adams [1975] p.11). For numerical purposes it may be preferable to use a Hilbert space, however the order of the Sobolev space to be used will be quite high for this problem (H^2 in one dimension (for $\alpha<\frac{1}{2}$) and of higher order in two or three dimensions - see Adams [1975] p.98).

We then have the following result.

THEOREM 3.4

There exists a solution to the minimization problem (3.42).

Proof From THEOREM 3.1 the Fréchet differentiability of the operator equation (3.41) follows - this implies continuity also. The problem is then one of minimizing a continuous functional over a compact set for which there exists a solution (THEOREM 1.4). □

We do not prove the continuous dependence of such solutions upon the measurement data, however a convergence result analogous to that of Colton and Kress [1983] p.238 could be proven (see §1.3.2).

The Miller-Tikhonov regularization technique has been applied to the inverse problem for their parabolic (time-varying) form of this equation by Kravaris and Seinfeld [1985] (see also Lee and Seinfeld [1987]). This inverse problem is an interior measurement problem and point measurements are utilized. Strong regularity theory is used (rather than our classical regularity theory) requiring only $f \in C^1(\overline{\Omega})$ rather than $f \in C^{1,\alpha}(\overline{\Omega})$. Some numerical results are presented for the reconstruction of a one-dimensional coefficient belong to a compact set

$$X_2 = \{f \in H^2(\Omega) : \|f\|_{H^2(\Omega)} \leq M \ , \ f \geq c > 0\}$$

i.e. a Sobolev space is utilized. A theorem for continuous dependence of solutions of the regularized inverse problem upon measurement data (that is a stability result) is also proven.

We note there is a strong regularity theory available for our elliptic equation as well - see Gilbarg and Trudinger [1983]. This requires $f \in C^1(\overline{\Omega})$ and gives existence, uniqueness and regularity for $\phi \in H^2(\Omega)$.

The regularization of such problems with Tikhonov's method is also discussed in Dietrich *et al.* [1988].

Andersson and Dietrich [1987] investigated an alternative approach for the regularization of the inverse problem of this chapter. This utilized the linear functional strategy and is based upon the weak form of the partial differential equation.

3.6 BOUNDARY MEASUREMENTS

The Fréchet differentiability result of THEOREM 3.1 may readily be extended to the case where $f\frac{\partial\phi}{\partial n}$, the normal flux (current) is measured on the boundary - with the Dirichlet boundary data being specified.

We set

$$\xi(f) = f\frac{\partial\phi(f)}{\partial n}\Big|_{\partial\Omega}$$

with

$$\phi(f) = g \ , \ \underset{\sim}{x} \in \partial\Omega \ .$$

THEOREM 3.5

The map $\xi : X_0 \rightarrow C^{1,\alpha}(\partial\Omega)$ is Fréchet differentiable with

$$\xi'(f)s = f\frac{\partial\phi'(f)s}{\partial n}\Big|_{\partial\Omega} + s\frac{\partial\phi(f)}{\partial n}\Big|_{\partial\Omega}$$

where $\phi'(f)s$ is given by (3.40).

<u>Proof</u> From THEOREM 3.1 $\phi(f)$ is Fréchet differentiable with the derivative (3.40). The differentiability of $\xi(f)$ with the above derivative follows using the chain rule - see COROLLARY 1.1. □

This result allows for either point measurements of $f\frac{\partial\phi}{\partial n}\Big|_{\partial\Omega}$ or measurements in $L^2(\partial D)$.

For this boundary measurement inverse problem the boundary data are usually chosen from a complete set. The normal flux, $f\frac{\partial\phi}{\partial n}$, may alternatively be specified as boundary data, with ϕ being measured on $\partial\Omega$.

However the Newton-Kantorovich method, for the determination of f, resulting from THEOREM 3.5 again requires the calculation of Green functions - see also Connolly [1985] and Connolly *et al.* [1985]. A more computationally efficient scheme for this problem is outlined in Connolly and Wall [1988] - which forms the Appendix. This paper also addresses questions such as uniqueness and stability for the boundary measurement inverse problem.

3.6.1 *Additional References*

We give here some additional recent references to work on the boundary measurement inverse problem (supplementing those in the Appendix).

Kohn and Vogelius [1987] investigate the relaxation of a variational method for the inverse problem. This suggests another iterative method for the solution of the inverse problem. They also conjecture the uniqueness of the solution of the inverse problem for arbitrarily smooth conductivities.

Friedman and Gustafsson [1987] consider reconstructing a conductivity of the form

$$f = 1 + k\chi_D$$

where χ_D is a characteristic function for D, an unknown subdomain. That is the shape of a conductivity anomaly is to be determined. They prove stability for the solution of the inverse problem with a suitable class of objects. We would expect that our methods for determining the shape of a scattering obstacle given in Chapter Four would be applicable here too.

Sylvester and Uhlmann [1988], for the original boundary measurement problem, establish the continuous dependence of the boundary values of the conductivity upon the potential to current maps. We note that this does not imply the continuous dependence of the solution of the inverse problem in the interior of the region. They also give a new proof of the theorem of Kohn and Vogelius [1984].

Continuous dependence is however proven for a regularized version of the inverse problem by Alessandrini [1988]. A constraint is placed upon $||f||_{H^4(\Omega)}$ (when n = 3) and a lower bound on f is also required. The continuity obtained is of logarithmic type, which we note is typical for problems with exponentially decaying singular values (see Betero *et al.* [1979]).

Finally Ramm [1988] proves uniqueness for solutions of this inverse problem for $f \in W^{1,\infty}(\Omega)$. To obtain this result the completeness of products of solutions of the p.d.e. is utilized.

CHAPTER FOUR

INVERSE BOUNDARY SCATTERING

4.1 INTRODUCTION

Scattering theory is concerned with solutions of the wave equation in exterior domains. This describes such phenomena as the scattering of acoustic and electromagnetic waves and also quantum mechanical scattering. In the frequency domain an equation describing this is the Helmholtz equation.

Inverse problems of considerable interest arise from the scattering of waves by an impenetrable obstacle. (Scattering by a refractive index for a penetrable object will be considered in Chapters Five and Six). The direct version is as follows. Suppose $\Omega \subset \mathbb{R}^n$, $n = 2,3$, is a bounded smooth domain. Given an incident field $u^i(\underset{\sim}{x})$ (which may have arisen from a time harmonic plane wave or a source distribution) determine

$$u(\underset{\sim}{x}) \in C^2(\mathbb{R}^n \backslash \overline{\Omega}) \cap C^1(\mathbb{R}^n \backslash \Omega)$$

such that

$$u(\underset{\sim}{x}) = u^i(\underset{\sim}{x}) + u^s(\underset{\sim}{x}), \quad \underset{\sim}{x} \in \mathbb{R}^n \backslash \Omega$$

$$\Delta u + k^2 u = 0 \quad \text{in } \mathbb{R}^n \backslash \overline{\Omega} \tag{4.1}$$

$$Bu = 0 \quad \text{on } \partial\Omega$$

and

$$\frac{\partial u^s}{\partial |\underset{\sim}{x}|} - iku^s \sim o(|\underset{\sim}{x}|)^{\frac{1-n}{2}}, \quad \text{as } \underset{\sim}{x} \to \infty .$$

B is a boundary operator and $Bu = 0$ represents either

(i) $u = 0$ on $\partial\Omega$, a Dirichlet boundary condition.

(ii) $\frac{\partial u}{\partial n} = 0$ on $\partial\Omega$, a Neumann boundary condition, or

(iii) $\frac{\partial u}{\partial n} + \lambda u = 0$ on $\partial\Omega$, an impedance boundary condition, where $\lambda = \lambda(\underset{\sim}{x})$ may vary along $\partial\Omega$.

The last condition of (4.1) is a radiation condition on the scattered field.

The scattered field has the following asymptotic behaviour

$$u^s(\underset{\sim}{x}) = \frac{e^{ik|\underset{\sim}{x}|}}{|\underset{\sim}{x}|^{(n-1)/2}} F\left(\frac{\underset{\sim}{x}}{|\underset{\sim}{x}|},k\right) + O(|\underset{\sim}{x}|^{-(n-1)/2})$$

where $F(\hat{\underset{\sim}{x}},k)$ is the farfield radiation pattern.

We shall consider two particular inverse problems for this scattering problem. Firstly, the boundary determination problem is examined. Here given knowledge of either the field on some surface exterior to Ω or the farfield pattern, $F(\hat{\underset{\sim}{x}},k)$, we wish to reconstruct the scattering boundary $\partial\Omega$. The other problem considered in §4.6 is the determination of a spatially varying impedance $\lambda(\underset{\sim}{x})$ on a given boundary, from knowledge of the farfield pattern. For reviews of these inverse problems the reader is referred to Sleeman [1982], Colton [1984] and Colton and Kress [1983].

We first outline previous theoretical and computational results available for the boundary determination problem. Then a result due to Angel *et al.* [1982] for the continuous dependence of farfield measurements upon the boundary is extended. We relax their requirement for the solution to belong to a compact set.

Unlike these authors we also use the implicit function theorem to obtain the continuous dependence result. This places this particular problem in the same class as the other problems of this thesis and illustrates the versatility of the approach.

We shall also compare various methods of computing the Fréchet derivative. In §4.4 we outline an approach via the null-field method which gives particularly straightforward equations to solve.

Finally for this problem in §4.5 we derive the partial differential equation satisfied by the Fréchet differential. An explicit expression for the Fréchet derivative is given and the relationship of this with the Hadamard variation is outlined.

In the last section of this chapter the impedance determination problem is considered. The continuous dependence of farfield measurements upon the impedance is established using the implicit function theorem. Fréchet differentiability of the map is also obtained.

In this introductory section we have not considered in very much depth the theory available for the direct problem. Particular methods of solution for this direct scattering problem will be outlined later before applying them to the solution of the corresponding inverse problem. Boundary integral equation methods for (4.1) are considered in detail in Colton and Kress [1983].

4.2 THE INVERSE PROBLEM

In this section we shall review what results are available for (i) the uniqueness of the boundary determination inverse problem, (ii) continuous dependence of the measurements upon the boundary, (iii) the stabilization of the inverse problem and, finally, (iv) the reconstruction of the boundary using iterative methods. We will consider in more detail some of these questions in following sections.

4.2.1 *Uniqueness*

The basic uniqueness result for this inverse problem is due to Schiffer. This states the scattering obstacle is uniquely determined by a knowledge of the farfield pattern F. As F is analytic in both $\hat{\underline{x}}$ and k, this may be reduced to knowing F for $\hat{\underline{x}}$ on some surface patch of the unit sphere and k on any interval of the positive real axis. The proof of Schiffer's theorem makes use of the properties of the eigenvalues and eigenfunctions of the Laplacian. However, it is nonconstructive and so of limited help in actually finding Ω.

We note that Colton and Sleeman [1983] have reduced the requirement for uniqueness to knowing the farfield pattern for a fixed value of the wavenumber and a finite number of different incident fields. Jones [1985] gives a proof of uniqueness applicable with a single incident field. For the details of Schiffer's result, see Lax and Phillips [1967] or Colton and Kress [1983] for example. This uniqueness result is extended to the elastodynamic case in Wall [1988b].

4.2.2 *Continuous Dependence*

Operator methods may also be applied to the solution of this particular inverse problem. The nonlinear operator equation formulation is

$$u[\partial\Omega] - U = 0 \ , \ \underline{x} \in M \tag{4.2}$$

where u is the direct problem solution and U the measurements available on a closed surface M exterior to and enclosing Ω. If instead farfield measurements are available, then the inverse problem may be expressed by an equation analogous to (4.2).

To solve this operator equation using iterative methods, its properties need to be investigated. In particular the continuous dependence of the field or farfield upon the scattering boundary must be established.

For the two-dimensional problem Colton and Kirsch [1981a] showed that if the boundary of the scattering obstacle is restricted to lie in a compact family of continuously differentiable curves, then the farfield depends continuously upon the boundary. Conformal mapping techniques are used in the proof of the result. The direct scattering problem is reformulated as an integral equation involving the conformal mapping taking the exterior of the disk onto the exterior of Ω. Having established the continuous dependence of the direct problem they then express the inverse problem as a minimization problem. The existence and stability of solutions of this problem is then proven.

Conformal mapping techniques are not available in $\mathbb{R}^3$. So to prove the corresponding result in three dimensions, Angell *et al.*[1982] reformulate the exterior Helmholtz boundary value problem in terms of an equivalent boundary integral equation.

There is a difficulty associated with the use of boundary integral equation methods for exterior boundary value problems. Even though the exterior boundary value problems for the Helmholtz equation are uniquely solvable for all wave numbers k with Im $k \geq 0$, the corresponding boundary integral equations fail to have unique solutions at eigenvalues of the adjoint interior problem, e.g. for second kind integral equations non-uniqueness results for the exterior Dirichlet problem at eigenvalues of the interior Neumann problem.

This difficulty is particularly significant in solving the inverse problem, as the location of the eigenvalues depends upon the shape of the boundary which is unknown. Thus a formulation of the boundary integral equations must be used which is uniquely solvable for all values of the wave number k, Im $k \geq 0$. Angell *et al.* use a technique with this uniqueness property in proving their results. It is assumed that the unknown scattering obstacle is strictly starlike with respect to the origin, i.e. $\partial\Omega$ can be parameterized in the form

$$\underset{\sim}{x} = f(\hat{\underset{\sim}{x}})\hat{\underset{\sim}{x}}$$

where f is a smooth function defined on the unit sphere. (Such an assumption was not necessary in the two dimensional results of Colton and Kirsch). They then show that if the function f belongs to a compact subset of the Hölder continuously differentiable functions, $C^{1,\alpha}$, then the farfield depends continuously upon the boundary. A stability result for the solution of the inverse problem is also proven in the paper for functions belonging to the compact subset.

As the imbedding $C^{1,\beta} \rightarrow C^{1,\alpha}$, $\beta > \alpha$ is compact, a suitable candidate for the compact set is a bounded subset of $C^{1,\beta}$, $\beta > \alpha$. For numerical purposes the use of a Hilbert space would be preferable, with a bounded subset of a Sobolev space, H^m, being chosen for the compact set. The value of m required to make the imbedding $H^m \rightarrow C^{1,\alpha}$ compact depends upon the dimension of the function f.

These continuity results are all proven in a direct manner without appealing to the implicit function theorem. Moreover, they find that the maps are in fact Hölder continuous. The proofs have similarities with that of Weston [1979] who proves Lipshitz continuity for the refractive index scattering problem. Weston also requires the unknown function to belong to a compact set.

This three dimensional theory is extended to the inverse transmission problem in Angell *et al.* [1987].

In the next section we investigate the application of the implicit function theorem to the three dimensional problem. We obtain continuous dependence results without the need to restrict the boundary to a compact set.

We note all this theory requires the surface to be continuously differentiable. There are difficulties presented by the scattering of waves by domains with corners - for example the loss of compactness of the associated integral operators (Colton and Kress [1983] p.31). In addition, an edge condition must be imposed on the solution - see Jones [1986] for example.

To prove such continuous dependence results, as well as having an integral equation formulation which is uniquely solvable for all wave numbers, the integral equation must have a bounded inverse. This requirement is analogous to that of ξ_y^{-1} being bounded in the implicit function theorem (see §1.5.3).

To date the integral equations utilized to obtain these results have been of the second kind, which for smooth enough boundaries have the desired property of boundedness of their inverse. For the two-dimensional problem Colton and Kirsch [1981a] used conformal mapping techniques to transform the inverse problem into a scattering problem with spatially varying refractive index on the exterior of a ball. An integral equation of the second kind was then obtained in a similar manner to Chapter Five. For the three dimensional problem, Angell *et al.* [1982] utilized a boundary integral equation of the second kind.

However, the alternative first kind boundary integral equation formulations have been shown to have bounded inverses (see Stephan [1987] and Wall [1988d]). This is provided suitable functions spaces are chosen for the data and solution - otherwise the integral operators may be compact.

4.2.3 *Construction of Solutions*

The first reconstructions for this problem using an iterative method were performed by Roger [1981]. The Newton-Kantorovich method is used to compute the shape of perfectly conducting cylinders. An integral equation of the first kind was used to solve the direct problem. The same author has also applied the technique to diffraction gratings - see Roger and Maystre [1979, 1980]. The regularization procedure employed essentially required constraints on the first derivative of the solution - that is, in the space $H^1[0,2\pi]$.

There are some reconstructions of a sound-soft obstacle in two-dimensions in Colton [1984] - these are due to Kirsch. Measurements of the total scattering cross section are used giving a comparatively simple expression for the Fréchet derivative from a variational principle due to Garabedian [1955]. The regularization theory outlined earlier is utilized with constraints

$$a \leq |f(\theta)| \leq b \quad \text{and} \quad |f''(\theta)| < C$$

being imposed on the starlike boundary for stability. Such a constraint arises as the imbedding $H^2[0, 2\pi] \rightarrow C^{1,\alpha}[0, 2\pi]$ is compact (for $\alpha < \frac{1}{2}$) for one dimensional functions.

Newton's method combined with the so-called null-field method for the direct problem has been examined in Wall *et al.* [1984] for an impenetrable obstacle. They obtain some preliminary numerical results when the boundary $\partial\Omega$ is characterized by a small number of parameters. The null-field method results in a generalized moment problem to solve the direct problem rather than a conventional integral equation. It has a unique solution for all frequencies (Colton and Kress [1983]) - with no difficulties at interior eigenvalues. As was noted earlier, this makes it particularly suitable for attacking the inverse problem where the boundary (and hence the interior eigenvalues) are unknown. We shall consider in more detail the derivative of the Fréchet derivative for the Newton-Kantorovich method via the null-field method in §4.4.

Kristensson and Vogel [1986] reconstruct some profiles in two dimensions using Newton's method and the null-field method. The Jacobian elements (Fréchet derivative) are computed by finite differences. We note the approach outlined by Wall *et al.* [1984] and is more computationally efficient as the Jacobian elements are actually computed in the direct problem solution.

Kristensson and Vogel use regularization methods and essentially add a constraint on the H^1 norm of the solution. This is weaker than the theory and numerical results in Colton [1984] which use a constraint on the H^2 norm of the solution. Quite reasonable results are obtained in the presence of measurement noise. The dimension of the approximating subspaces, N (i.e. the number of basis functions used for the solution) is large enough so that the stabilization is due to the inversion method and not the size of N. Roger [1981] also only required a constraint on the H^1 norm of the solution.

Colton and Monk [1985, 1986] present an alternative method for solving the inverse problem - though still based upon nonlinear optimization. This method is developed in the first paper for the case where the farfield is known for an interval of frequency values. This is extended in the second paper to when the farfield is known at only one frequency.

They use the theory of Herglotz wave functions to obtain a minimization problem having a very simple Fréchet derivative. The approach avoids the use of integral equations. To minimize the functional, optimization methods must still be used. Some numerical results with a quasi-Newton method are presented.

The approach is applicable to both scattering by both hard and soft obstacles. The authors are of the opinion their scheme provides an efficient and practical method for the inverse scattering problem. However, the authors note a disadvantage of their method is the need to know both the amplitude and phase. When the phase is unknown and only the amplitude is measured, we must solve the conventional operator equation (4.2) - that is, find an obstacle such that the corresponding farfield data best fits the measured data (see §6.2.3).

We also note that this approach was applied to an inverse transmission problem in Colton and Monk [1987]. It was utilized to determine the boundary of a penetrable obstacle with constant refractive index.

4.2.4 *Vector Problems*

There is also interest in solving inverse boundary scattering problems for linear elasticity and vector Helmholtz equations. Uniquely solvable boundary integral equations have been devised for the direct problems - see Colton and Kress [1983] for the vector Helmholtz equation and Jones [1984b] for the linear elasticity equation. Existence is proven for the equations in Colton and Kress using Fredholm theory. The integral operators involved have strong singularities but are transformed into compact operators.

Little has been done on the inverse boundary scattering problems for these two equations. However, Colton and Kress [1983] do prove uniqueness results for determining either the boundary or an impedance boundary condition on it for the vector Helmholtz equation. Uniqueness for elastodynamic inverse boundary scattering is proven in Wall [1988b].

4.3 IMPLICIT FUNCTION THEOREM

We shall prove a continuous dependence result for the boundary to farfield map. A boundary integral formulation of the problem is used to show the map is continuous for a Hölder continuously differentiable and starlike boundary. We make use of the work of Angell, Colton and Kirsch [1982]. However, our approach differs in several respects - both in the final result and the method of proof for which we utilize the implicit function theorem. We also examine the Fréchet derivative of the boundary to field map that is obtained.

4.2.1 *Boundary Integral Equation*

Let $\Gamma_0 = \{\underset{\sim}{x} \in \mathbb{R}^3 : |\underset{\sim}{x}| = 1\}$ denote the surface of the unit ball in $\mathbb{R}^3$ and let $C^{1,\alpha}(\Gamma_0)$ denote the space of Hölder continuously differentiable functions. We will assume the scatterer is starlike and is described by

$$\Gamma(f) = \{\underset{\sim}{x} \in \mathbb{R}^3 : \underset{\sim}{x} = f(\hat{\underset{\sim}{x}})\hat{\underset{\sim}{x}} \, , \, \hat{\underset{\sim}{x}} = \underset{\sim}{x}/|\underset{\sim}{x}|\}$$

where $f : \Gamma_0 \to \mathbb{R}^3$ belongs to $C^{1,\alpha}(\Gamma_0)$. The function f will be required to belong to the subset

$$X_0 = \{f \in C^{1,\alpha}(\Gamma_0) : \|f\|_{1,\alpha} < M, \, f(\hat{\underset{\sim}{x}}) < a, \, \hat{\underset{\sim}{x}} \in \Gamma_0\}$$

A surface described by such a function contains a ball, B_a, of radius a.

The direct scattering problem is then for each $f \in X_0$ solve

$$\begin{aligned} u(\underset{\sim}{x}) &= u^i(\underset{\sim}{x}) + u^s(\underset{\sim}{x}) \qquad\qquad (4.3) \\ \Delta u(\underset{\sim}{x}) + k^2 u(\underset{\sim}{x}) &= 0 \ , \ \underset{\sim}{x} \text{ outside } \Gamma(f) \\ u(\underset{\sim}{x}) &= 0 \ , \ \underset{\sim}{x} \in \Gamma(f) \end{aligned}$$

and $\quad u^s(\underset{\sim}{x})$ satisfies the radiation condition.

We shall show that the map from $f \in X_0$ to the farfield F(f) is continuous. We shall make use of some intermediate results due to Angell, Colton and Kirsch [1982] who prove the same result, but for a compact subset of X_0, using a different method. We shall make use of the implicit function theorem and need only boundedness of the subset and not a compactness assumption.

We require a uniquely solvable boundary integral equation formulation. Like Angell *et al* [1982] we use a technique due to Ursell [1973] and look for a solution u^s in the form of a double layer potential density ψ.

$$u^s(\underset{\sim}{x}) = \int_{\Gamma(f)} \left[\frac{\partial}{\partial n_y} G(\underset{\sim}{x}, \underset{\sim}{y})\right] \psi(\underset{\sim}{y}) d\underset{\sim}{y} \, , \, \underset{\sim}{x} \in \mathbb{R}^3 \ .$$

Here $\frac{\partial}{\partial n_y}$ denotes differentiation in the direction of the unit normal to the surface $\Gamma(f)$ at the point $y \in \Gamma(f)$ pointing into the exterior of $\Gamma(f)$. G is the Helmholtz

Green's function for the exterior of the ball B_a, satisfying a dissipative boundary condition on ∂B_a. This Green's function can be written in the form

$$G(\underset{\sim}{x},\underset{\sim}{y}) = - \frac{e^{ik|\underset{\sim}{x}-\underset{\sim}{y}|}}{2\pi|\underset{\sim}{x}-\underset{\sim}{y}|} + G_1(\underset{\sim}{x},\underset{\sim}{y})$$

where G_1 is a continuous wave function.

The unknown density ψ satisfies the Fredholm integral equation of the second kind on $\Gamma(f)$

$$\psi(\underset{\sim}{x}) - \int_{\Gamma(f)} \left[\frac{\partial}{\partial n_y} G(\underset{\sim}{x},\underset{\sim}{y})\right] \psi(\underset{\sim}{y})d\underset{\sim}{y} + u^i(\underset{\sim}{x}) = 0, \; \underset{\sim}{x} \in \Gamma(f). \tag{4.4}$$

This integral equation is uniquely solvable for all values of k, Im k $\geq$ 0 provided the exterior boundary value problem itself has a unique solution (Ursell [1973]).

We wish to study the map $f \rightarrow F(f)$ from the boundary to the farfield. To do this we must first examine the map $f \rightarrow \psi$ from X_0 into $C^0(\Gamma_0)$.

Consider the following integral equation obtained by means of the change of variables $\underset{\sim}{x} = f(\hat{\underset{\sim}{x}})\hat{\underset{\sim}{x}}$

$$\psi(f(\hat{\underset{\sim}{x}})\hat{\underset{\sim}{x}}) - \int_{\Gamma_0} \frac{\partial}{\partial n_y} \left[G(f(\hat{\underset{\sim}{x}})\hat{\underset{\sim}{x}}, f(\hat{\underset{\sim}{y}})\hat{\underset{\sim}{y}})\right] \psi(f(\hat{\underset{\sim}{y}})\hat{\underset{\sim}{y}}) J_f(\hat{\underset{\sim}{y}})d\hat{\underset{\sim}{y}}$$

$$= - u^i(f(\hat{\underset{\sim}{x}})\hat{\underset{\sim}{x}}) \qquad (4.5)$$

where J_f is the Jacobian of the transformation.

Introducing the functions $\varphi(\hat{\underset{\sim}{x}}) = \psi(f(\hat{\underset{\sim}{x}})\hat{\underset{\sim}{x}})$, $v_f(\hat{\underset{\sim}{x}}) = - u^i(f(\hat{\underset{\sim}{x}})\hat{\underset{\sim}{x}})$, and

$$a_f(\hat{\underset{\sim}{x}},\hat{\underset{\sim}{y}}) = - \frac{\partial}{\partial n_y}[G(f(\hat{\underset{\sim}{x}})\hat{\underset{\sim}{x}}) , f(\hat{\underset{\sim}{y}})\hat{\underset{\sim}{y}}] \, J_f(\hat{\underset{\sim}{y}})$$

this may be written as

$$\varphi(\underset{\sim}{x}) + \int_{\Gamma_0} a_f(\hat{\underset{\sim}{x}},\hat{\underset{\sim}{y}})\, \rho(\hat{\underset{\sim}{y}})d\hat{\underset{\sim}{y}} = v_f(\hat{\underset{\sim}{x}})\,, \quad \hat{\underset{\sim}{x}} \in \Gamma_0$$

or

$$\varphi + A_f\, \varphi = v_f \ .$$

Each choice of $f \in X_0$ yields a unique function $\varphi(f;\hat{\underset{\sim}{x}})$ which is a solution of this equation.

4.3.2 *Continuous Dependence*

The equation is now in the form $\xi(v, y(v)) = 0$ and the implicit function theorem may be applied to show that the map $f \rightarrow \varphi(f)$ from X_0 into $C^0(\Gamma_0)$ is continuous.

First we need the following lemma on the properties of A_f.

LEMMA 4.1 For any $\delta \leq \frac{1}{2}(1-\alpha)$, there exists a constant Y such that

(a) $|a_f(\hat{\underset{\sim}{x}},\hat{\underset{\sim}{y}})| \leq \gamma|\hat{\underset{\sim}{x}}-\hat{\underset{\sim}{y}}|^{\alpha-2}$, for all $\hat{\underset{\sim}{x}},\hat{\underset{\sim}{y}} \in \Gamma_0$ and $f \in X_0$.

(b) $|a_f(\hat{\underset{\sim}{x}},\hat{\underset{\sim}{y}})| - a_g(\hat{\underset{\sim}{x}},\hat{\underset{\sim}{y}}) \leq \gamma|\hat{\underset{\sim}{x}}-\hat{\underset{\sim}{y}}|^{\alpha-2}||f-g||^{\delta}_{1,\alpha}$ for all $\hat{\underset{\sim}{x}},\hat{\underset{\sim}{y}} \in \Gamma_0$ and $f \in X_0$.

<u>Proof</u>: See Angel *et al.*[1982], pp.51-52. □

Part (a) establishes the weakly singular nature of the kernels a_f, and (b) their continuous dependence upon f.

THEOREM 4.2

Assume that the map $f \to v_f$ from $X_0 \to C^0(\Gamma_0)$ is continuous. Then t

maps

(i) $\quad f \to \varphi(f) \quad$ from $\quad X_0 \to C^0(\Gamma_0)$

and (ii) $\quad f \to F(f) \quad$ from $\quad X_0 \to C^0(\Gamma_0)$

are continuous.

<u>Proof</u> (i) Set $\xi(f,\varphi) = \varphi - A_f\varphi - v_f$

$$= \varphi(\hat{\underset{\sim}{x}}) + \int_{\Gamma_0} a_f(\hat{\underset{\sim}{x}},\hat{\underset{\sim}{y}})\, \varphi(\hat{\underset{\sim}{y}})\, d\hat{\underset{\sim}{y}} - v_f(\hat{\underset{\sim}{x}}), \quad \hat{\underset{\sim}{x}} \in \Gamma_0 \ .$$

Then $\xi : X_0 \otimes C^0(\Gamma_0) \to C^0(\Gamma_0)$.

We shall check the conditions of the implicit function theorem (THEOREM 1.1).

1. ξ is continuous.

We have

$$\begin{aligned}
\delta\xi &= \xi(f + \delta f, \varphi + \delta\varphi) - \xi(f,\varphi) \\
&= \varphi(\hat{\underset{\sim}{x}}) + \delta\varphi(\hat{\underset{\sim}{x}}) + \int_{\Gamma_0} a_{f+\delta f}(\hat{\underset{\sim}{x}},\hat{\underset{\sim}{y}})[\varphi(\hat{\underset{\sim}{y}}) + \delta\varphi(\hat{\underset{\sim}{y}})]\, d\hat{\underset{\sim}{y}} - v_{f+\delta f}(\hat{\underset{\sim}{x}}) \\
&\quad - [\varphi(\hat{\underset{\sim}{x}}) + \int_{\Gamma_0} a_f(\hat{\underset{\sim}{x}},\hat{\underset{\sim}{y}})\, \varphi(\hat{\underset{\sim}{y}})\, d\hat{\underset{\sim}{y}} - v_f(\hat{\underset{\sim}{x}})] \\
&= \delta\varphi(\hat{\underset{\sim}{x}}) + \int_{\Gamma_0} [a_{f+\delta f}(\hat{\underset{\sim}{x}},\hat{\underset{\sim}{y}}) - a_f(\hat{\underset{\sim}{x}},\hat{\underset{\sim}{y}})]\, [\varphi(\hat{\underset{\sim}{y}}) + \delta\varphi(\hat{\underset{\sim}{y}})] d\hat{\underset{\sim}{y}} \\
&\quad + \int_{\Gamma_0} a_f(\hat{\underset{\sim}{x}},\hat{\underset{\sim}{y}})\, \delta\varphi(\hat{\underset{\sim}{x}}) d\hat{\underset{\sim}{y}} + v_f(\hat{\underset{\sim}{x}}) - v_{f+\delta f}(\hat{\underset{\sim}{x}}) \ .
\end{aligned}$$

This gives

$$|\delta\xi(\hat{\underset{\sim}{x}})| \leq |\delta\varphi(\hat{\underset{\sim}{x}})| + \|\varphi + \delta\varphi\|_\infty \int_{\Gamma_0} |a_{f+\delta f}(\hat{\underset{\sim}{x}},\hat{\underset{\sim}{y}}) - a_f(\hat{\underset{\sim}{x}},\hat{\underset{\sim}{y}})|\, d\hat{\underset{\sim}{y}}$$

$$+ \|\delta\varphi\|_\infty \int_{\Gamma_0} |a_f(\hat{\underset{\sim}{x}},\hat{\underset{\sim}{y}})|\, d\hat{\underset{\sim}{y}} + |v_{f+\delta f}(\hat{\underset{\sim}{x}}) - v_f(\hat{\underset{\sim}{x}})| \ .$$

So
$$\|\delta\xi\|_\infty \leq \|\delta\varphi\|_\infty + \alpha(\|\varphi\|_\infty + \|\delta\varphi\|_\infty)\, \|\delta f\|^{\delta}_{1,\alpha}$$
$$+ \beta\|\delta\varphi\|_\infty + \|v_{f+\delta f} - v_f\|_\infty \ .$$

As $\|\delta f\|_{1,\alpha} \to 0$, $\|v_{f+\delta f} - v_f\|_\infty \to 0$ so that
$\|\delta\xi\|_\infty \to 0$ as $\|\delta f\|_{1,\alpha}$, $\|\delta\varphi\|_\infty \to 0$

i.e. ξ is continuous in f and φ.

2. $\xi_\varphi(f,\varphi)$ is continuous.

Now

$$\xi_\varphi(f,\varphi)s = s + A_f s.$$

This gives

$$\begin{aligned} \|\xi_\varphi(f+\delta f, \varphi+\delta\varphi) - \xi_\varphi(f,\varphi)\|_\infty &= \|(A_{f+\delta f} - A_f)s\| \\ &\leq \alpha\|\delta f\|^{\delta}_{1,\alpha}\, \|s\|_\infty \end{aligned}$$

from 1.

Thus $\xi_\varphi(f,\varphi)$ is continuous in f and φ as required.

3. $[\xi_\varphi(f,)]^{-1}$ is bounded.

We have

$$[\xi_\varphi(f,\varphi)]^{-1} = (I + A_f)^{-1}.$$

Now $A_f : C^0(\Gamma_0) \rightarrow C^0(\Gamma_0)$ is compact (it is an operator with weak singularity) and a solution of the integral equation is unique. So from the Fredholm alternative theorem $(I + A_f)^{-1}$ is bounded.

So all the conditions of the implicit function theorem are satisfied and the map $f \rightarrow \varphi(f)$ is continuous.

(ii) We wish to show $f \rightarrow F(f)$ is continuous, i.e. the farfield depends continuously upon the boundary. This follows from the result of (i) in a similar manner to Angell *et al.* [1982]. □

So in summary, we have proven continuity of the map for $f \in C^{1,\alpha}$, $||f||_{1,\alpha} < M$ and $f > a$ using the implicit function theorem. On the other hand, Angell *et al.* [1982] proved Hölder continuity for a compact subset, X_1, of this set. They did this by showing the operators $(I + A_f)^{-1}$, $f \in X_1$ were equibounded.

So we can remove the compactness of the subset and still obtain continuity, however we may lose the Hölder nature of this continuity.

In summary the problem was transformed from determining the boundary of a region on which a partial differential equation is defined, into determining a coefficient function in an integral equation. The problem was then in the form $\xi(v,y(v)) = 0$ and the implicit function theorem was applicable. The inverse boundary scattering problem then became of the same class as the other inverse problems we have considered. This also illustrates the versatility of the implicit function theorem for proving continuity of nonlinear operator equation formulations for inverse problems.

4.3.3 *The Frechet Derivative*

Having established the continuous dependence of the density and far-field upon the boundary we now examine the Fréchet derivative. We note Angell *et al.*

[1982] do not consider the existence of this Fréchet derivative.

The function $\varphi(f)$ satisfies

$$\varphi(f) + A_f\varphi(f) = v_f \quad .$$

Differentiating with respect to f gives

$$\varphi'(f)s + A_f\varphi'(f)s + A_f\ \varphi(f)s = v_f' s$$

or

$$\varphi'(f)s = [I + A_f]^{-1}(v_f' s - A_f' \varphi(f)s).$$

We have already established the existence of $[I + A_f]^{-1}$ and shall now investigate the derivative of the kernel A_f' in more detail.

The quantity $\varphi(f:\hat{\underline{x}})$ satisfies the following integral equation

$$\varphi(f;\hat{\underline{x}}) - \int_{\Gamma_0} \frac{\partial}{\partial n_y}[G(f(\hat{\underline{x}})\hat{\underline{x}}, f(\hat{\underline{y}})\hat{\underline{y}})\ \varphi(f;\hat{\underline{y}})J_f(\hat{\underline{y}})d\hat{\underline{y}}$$

$$= - u^i(f(\hat{\underline{x}})\hat{\underline{x}}), \quad \hat{\underline{x}} \in \Gamma_0 \ . \tag{4.6}$$

We wish to obtain the equation satisfied by the Fréchet differential $\varphi'(f)s$.

Using the Taylor expansion

$$\xi(\underline{f} + \underline{s}) - \xi(\underline{f}) = \underline{s}\cdot\nabla\xi(\underline{f}) \quad \text{for small } \underline{s}\,,$$

we obtain the following linearizations.

$$G((f+s)(\hat{\underline{x}})\hat{\underline{x}}, (f+s)(\hat{\underline{y}})\hat{\underline{y}}) - G(f(\hat{\underline{x}})\hat{\underline{x}}, f(\hat{\underline{y}})\hat{\underline{y}}) = \hat{\underline{x}}\cdot\nabla_x G(f(\hat{\underline{x}})\hat{\underline{x}}, f(\hat{\underline{y}})\hat{\underline{y}})s(\hat{\underline{x}})$$
$$+ \hat{\underline{y}}\cdot\nabla_y G(f(\hat{\underline{x}})\hat{\underline{x}},f(\hat{\underline{y}})\hat{\underline{y}})s(\hat{\underline{y}})$$

and

$$u^i((f+s)(\hat{\underline{x}})\hat{\underline{x}}) - u^i(f(\hat{\underline{x}})\hat{\underline{x}}) = \hat{\underline{x}} \cdot \nabla_x u^i(f(\hat{\underline{x}})\hat{\underline{x}}) s(\hat{\underline{x}})$$

So that differentiating (4.6) with respect to f gives

$$\varphi'(f)s - \int_{\Gamma_0} \frac{\partial}{\partial n_y} \left[G(f(\hat{\underline{x}})\hat{\underline{x}}, f(\hat{\underline{y}})\hat{\underline{y}} \right] J_f(\hat{\underline{y}})\, \varphi'(f)s \, d\hat{\underline{y}}$$

$$= \int_{\Gamma_0} \frac{\partial}{\partial n_y} \left[G(f(\hat{\underline{x}})\hat{\underline{x}}, f(\hat{\underline{y}})\hat{\underline{y}}) \right] \varphi(f;\hat{\underline{y}})\, J_f'(\hat{\underline{y}}) s(\hat{\underline{y}}) d\hat{\underline{y}}$$

$$+ \int_{\Gamma_0} \frac{\partial}{\partial n_y} \left[\hat{\underline{x}} \cdot \nabla_x G(f(\hat{\underline{x}})\hat{\underline{x}}, f(\hat{\underline{y}})\hat{\underline{y}})\, s(\hat{\underline{x}}) \right] \varphi(f;\hat{\underline{y}})\, J_f(\hat{\underline{y}}) d\hat{\underline{y}}$$

$$+ \int_{\Gamma_0} \frac{\partial}{\partial n_y} \left[\hat{\underline{y}} \cdot \nabla_y G(f(\hat{\underline{x}})\hat{\underline{x}}, f(\hat{\underline{y}})\hat{\underline{y}}) \right. \varphi(f;\hat{\underline{y}})\, J_f(\hat{\underline{y}}) s(\hat{\underline{y}}) d\hat{\underline{y}}$$

$$- \hat{\underline{x}} \cdot \nabla u^i(f(\hat{\underline{x}})\hat{\underline{x}})\, s(\hat{\underline{x}}) \quad , \quad x \in \Gamma_0 \, .$$

Taking the operations involving x outside the third integral gives

$$\underline{s}(\hat{\underline{x}})\, \hat{\underline{x}} \cdot \nabla_x \int_{\Gamma_0} \frac{\partial}{\partial n_y} \left[G(f(\hat{\underline{x}})\hat{\underline{x}}, f(\hat{\underline{y}})\hat{\underline{y}}) \right] \varphi(f;\hat{\underline{y}})\, J_f(\hat{\underline{y}}) d\hat{\underline{y}}$$

$$= s(\hat{\underline{x}})\, \hat{\underline{x}} \cdot \nabla_x\, u^i(f(\hat{\underline{x}})\hat{\underline{x}}) + s(\hat{\underline{x}})\, \hat{\underline{x}} \cdot \nabla_x \varphi(f;\hat{\underline{x}})$$

from (4.6).

Hence we may replace the second term in the right hand side of (4.7) by $\hat{\underline{x}} \cdot \nabla_x \varphi(f;\hat{\underline{x}})\, s(\hat{\underline{x}})$ and drop the last term. This simplifies the equations slightly.

However, we still have the third term present. This contains two y derivatives on G and so contains a strong singularity. Thus unless this term can be eliminated it is not clear that A_f' exists as it stands. For the implicit function theorem to give Fréchet differentiability as well as continuity $\xi_f(f,\varphi)$ must exist. However, it may well be possible to overcome this strong singularity using Fredholm operator theory and the symbol of the operator.

It should be noted that Roger [1981] in deriving the Fréchet derivative via a first kind integral equation formulation also obtained integral operators with strong singularities. Alternatively, if we use the null-field method to derive the Fréchet derivative (see §4.4) then the equations obtained do not have such difficulties with singularities. Also as in a first kind integral formulation the Jacobian may be combined with the density, this simplifies things a little. In a second kind integral equation the density also appears outside the integral and so cannot be combined with the Jacobian.

Due to the complicated nature of the Fréchet derivative for this particular problem, several authors when performing some numerical reconstructions, instead of knowlege of the farfield or its amplitude, utilize the total scattering cross section

$$\sigma(f) = \int_{\Gamma_0} |F(f;\hat{\underline{x}})|^2 d\hat{\underline{x}} \ . \tag{4.8}$$

Here $F(f;\hat{\underline{x}})$ is the farfield pattern resulting from incident field $u^i = \exp(ik\underline{x}\cdot\underline{\alpha})$ and boundary given by f.

To compute the Fréchet derivative they make use of the Hadamard variation given by Garabedian [1955]

$$\delta\sigma = -\operatorname{Im}\frac{1}{k}\int_{\Gamma(f)} \frac{\partial u_-(f;\underline{x})}{\partial n} \frac{\partial u_+(f;\underline{x})}{\partial n} \delta n \, ds \ . \tag{4.9}$$

The quantity δn is a small shift along the inner normal to $\partial\Omega$. The functions u_+ and u_- are the solutions of the direct problem with u^i given by $\exp(ik\underline{x}\cdot\underline{\alpha})$ and $\exp(-ik\underline{x}\cdot\underline{\alpha})$ respectively. In this case we may obtain an explicit expression for the Fréchet differential rather than an integral equation which it satisfies.

We are not aware of a formal proof of Fréchet differentiability even for $\sigma(f)$, based upon this variational principle, in appropriate function spaces. It should however be possible to extend the result of Colton and Kirsch [1981a] for the continuity of the boundary to farfield map into a Fréchet differentiability result. Conformal mapping techniques are used and the difficulty with a strongly singular integral operator resulting from the boundary integral formulation would be avoided. We note the result requires the solution to belong to a compact subset of continuously differentiable curves and also that the implicit function theorem is not utilized.

In §4.5 we obtain the partial differential equation satisfied by the Fréchet differential resulting from a starlike scatterer. An explicit expression for the Fréchet derivative is then obtained and also its relationship with the Hadamard variation of the field examined. The derivation is informal in nature and so we do not prove the existence of this Fréchet derivative.

4.4 NULL FIELD METHOD

In this section we examine the solution of the inverse problem via the null field method (Bates and Wall [1977]) of solution for the direct scattering problem. We shall find that the equations obtained for the Newton-Kantorovich method are fairly straightforward compared with the expressions obtained for the Fréchet derivative in the last section. Also much of the work necessary for solving them has been performed in the direct problem solution.

As was noted earlier, Wall *et al.* [1985], Kristensson and Vogel [1986] and Murch, Tan and Wall [1988] have used the null field method combined with Newton's method to obtain solutions of the inverse boundary scattering problem. However, the derivations in the first and third papers are in finite dimensional spaces and the second paper uses differences to compute the derivatives. We shall obtain Newton's method in infinite dimensional space.

The null field method is particularly suitable for solving the inverse problem as it has a unique solution for all frequencies. The null field method also holds much promise for solving the corresponding elastodynamic inverse problem, where there are difficulties with singularities in the conventional boundary integral equation methods of solution.

4.4.1 *Direct Problem Solution*

We shall consider the solution of the direct problem in two dimensions with the null field method. The boundary $\partial\Omega$ is required to be smooth and starlike - and so can be represented by a single-valued function of the polar angle, $r(\theta)$.

The incident wave can be written in the multipole expansion

$$u^i = \sum_{n=-\infty}^{\infty} a_n J_n(kr) \exp(in\theta) \ ,$$

where the $\{a_n\}$ are known coefficients of the wave and J_n denotes the Bessel function of order n.

The null field equations of this direct scattering problem with Dirichlet boundary data are

$$\int_0^{2\pi} f(\theta)\, H_n^{(1)}(kr(\theta)) \exp(in\theta) d\theta = a_n \, , \ n \in \mathbb{Z} \qquad (4.10)$$

where

$$f(\theta) = \hat{\underline{n}} \cdot \nabla u(\underline{x}) \left[1 + \left[\frac{1}{r} \frac{dr}{d\theta} \right]^2 \right]^{\frac{1}{2}} \cdot \frac{i}{4} \, , \; \underline{x} \in \partial\Omega$$

is the normalized source density.

$H_n^{(1)}$ denotes the Hankel function of the first kind of order n and $\hat{\underline{n}}$ is the outward normal to $\partial\Omega$. The above equation is a moment problem and so can be solved numerically by means of a basis function expansion

$$f(\theta) = \sum_{m=1}^{N} c_m f_m(\theta) \; .$$

Generally regularization techniques will be required in solving the moment problem.

The asymptotic behaviour of the scattered field u^S as $r \to \infty$ is

$$u^S(\underline{x}) = r^{-\frac{1}{2}} \exp(ikr) \, F(\theta) + O(r^{-1}) \; .$$

$F(\theta)$ is the scattering amplitude and is given by

$$F(\theta) = - \sum_{n=-\infty}^{\infty} (i)^n \, b_n \exp(im\theta)$$

where

$$b_n = \int_0^{2\pi} f(\theta) \, J_n(kr(\theta)) \exp(in\theta) d\theta \, , \; n \in \mathbb{Z} \; . \qquad (4.11)$$

As $J_n = \mathrm{Re}(H_n^{(1)})$ the appropriate quadratures for computing the b_n have already been evaluated while solving the moment problem (4.10).

4.4.2 *Newton–Kantorovich Method*

We shall assume that the farfield (and hence the b_n) is known. Our methods can easily be modified for the case where only the amplitude of the farfield is measured.

The farfield and density are functionals of the boundary so that

$$b_n = b_n(r(\theta)) \quad \text{and} \quad f(\theta) = f(r(\theta); \theta) \; .$$

The operator equation to be solved is

$$T(r) = b_n(r) - \breve{b}_n = 0 \, , \; n \in \mathbb{Z} \tag{4.12}$$

where the $\{\breve{b}_n\}$ result from the measured values of the farfield.

The Fréchet derivative $b_n'(r)$ is computed from the direct problem formulation

$$b_n(r) = \int_0^{2\pi} f(r;\theta) \, J_n(kr(\theta)) \exp(in\theta) d\theta \tag{4.13}$$

and

$$a_n = \int_0^{2\pi} f(r;\theta) \, H_n^{(1)}(kr(\theta)) \exp(in\theta) d\theta \; . \tag{4.14}$$

Differentiating these equations with respect to $r(\theta)$ gives

$$b_n'(r)s = \int_0^{2\pi} \left[f'(r)s \, J_n(kr(\theta) + kf(r(\theta)) \, J_n' \quad (kr(\theta))s(\theta) \right] e^{in\theta} d\theta \tag{4.15}$$

and

$$0 = \int_0^{2\pi} \left[f'(r)s\, H_n^{(1)}(kr(\theta)) + kf(r(\theta))\, H_n^{(1)\prime}(kr(\theta)\right] e^{in\theta} d\theta\,, \qquad n \in \mathbb{Z}\,. \tag{4.16}$$

Here $f'(r)$ is the Fréchet derivative of the density.

In the Newton-Kantorovich method the equation

$$b_n'(r^{(k)})s^{(k)} = \tilde{b}_n - b_n(r^{(k)})\,,\ n \in \mathbb{Z}$$

must be solved for the update $s^{(k)}$. This gives

$$\int_0^{2\pi} \left[f'(r^{(k)})s^{(k)}\, J_n\left[kr^{(k)}(\theta)\right] + kf(r^{(k)}(\theta))\, J_n' \left[kr^{(k)}(\theta)\right] s^{(k)}(\theta)\right] e^{in\theta} d\theta = \tilde{b}_n - b_n\left[r^{(k)}\right] \tag{4.17}$$

$$\int_0^{2\pi} \left[f'(r^{(k)})s^{(k)}\, H_n^{(1)}\left[k(r^{(k)}(\theta)\right] + kf(r^{(k)}(\theta))\, H_n^{(1)\prime}\left[kr^{(k)}(\theta)\right] s^{(k)}(\theta)\right] e^{in\theta} d\theta = 0\,,\ n \in \mathbb{Z}\,. \tag{4.18}$$

That is at each iteration a 2 x 2 system of moment problems must be solved for the quantities $f'(r^{(k)})s^{(k)}$ and $s^{(k)}$. We cannot see any way of eliminating the intermediate quantity $f'(r^{(k)})s^{(k)}$.

The system of equations to be solved is clearly very similar in form to the direct problem itself. This means a lot of the work in evaluating integrals was performed in the direct problem solution. So it makes sense to implement the Newton-Kantorovich method in this manner rather than computing the derivatives by differences as Kristensson and Vogel [1986] do. In fact, Murch *et al.* [1988] utilized a finite dimensional analogue of equations (4.17) and (4.18) to obtain their reconstructions.

Due to the possibly ill-conditioned nature of the matrix equations obtained, regularization methods must be used to solve the inverse problem. From the similarity in form of the equations to those defining the direction problem, the same regularization scheme could be used for the inverse problem.

However we would expect to use a much larger value of the regularization parameter in solving the inverse problem. This is because in the direct problem the right hand side of the equation, a_n, is known exactly, and the errors result from the numerical procedure. However in the inverse problem, the right hand side $\tilde{b}_n$ is subject to measurement noise.

We note that when the boundary is a circle, and a Fourier series expansion is performed on f, the null field method reduces to a diagonal system of equations to solve for the Fourier coefficients and hence f.

So in the case of the linearization of the operator equation about $r(\theta) = r_0$, a constant, (that is a circular boundary) we can then actually determine from (4.18) an explicit expression for $f'(r_0)s$ in terms of $s(\theta)$. Substituting this into (4.17) gives a *single* moment problem to solve in this case. This may be of use in solving the problem when we know the boundary is a small perturbation on a circle or alternatively if the modified form of the Newton-Kantorovich method is utilized.

Numerical results with the null field method combined with the Newton-Kantorovich method have been obtained by Wall *et al.* [1985], Kristensson and Vogel [1986] and Murch *et al.* [1988]. Wall *et al.* [1985] computed the radius of a circular cylinder from knowledge of the scattering cross-section. Kristensson and Vogel [1986] reconstructed a range of different objects (including non-convex ones) in both the cases where the phase of the scattered field is known and unknown. Regularization techniques were also incorporated. Murch *et al.* also reconstructed a non-convex object, with the computations being performed in an efficient manner - the Fréchet derivative was computed from the direct problem solution. They considered the Neumann problem in addition to the Dirichlet one. Kristensson and Vogel used finite differences to estimate the Fréchet derivative - requiring the use of a CRAY X-MP for the computations.

4.5 THE FRÉCHET DERIVATIVE

In this chapter we have so far examined methods of computing the Fréchet derivative of the boundary to field map via several different formulations of the direct problem. These include Fredholm boundary integral equations of the second kind and the null-field method. We now derive via variational methods the partial differential equation satisfied by the Fréchet differential. This equation is found to be of the same form as the direct problem - so we can then use any direct problem formulation desired to compute this Fréchet derivative.

It is also possible to obtain an explicit formula for the Fréchet derivative from the equation it satisfies using an appropriate Green's function. Throughout this section the scatterer is assumed to be starlike.

4.5.1 *Variational Approach*

Let $\Omega_{f+\delta f}$ be obtained from Ω_f by a small shift (inwards or outwards) $\delta f(\theta)$ in the radial direction in $\mathbb{R}^2$ or $\mathbb{R}^3$. Let $u + \delta u$ be the resulting solution of the Helmholtz equation, so that δu is the change in the solution due to a change δf in the boundary.

Now

$$\Delta(u+\delta u) + k^2(u+\delta u) = 0 \quad \text{in } \mathbb{R}^n \backslash \Omega_{f+\delta f}$$

and $\qquad u+\delta u - u^i$ satisfies the radiation condition.

If δf is small enough then $u + \delta u$ satisfies the Helmholtz equation in the exterior of Ω_f as well. So

$$\Delta(u+\delta u) + k^2(u+\delta u) = 0 \quad \text{in} \quad \mathbb{R}^n\backslash\Omega_f.$$

But

$$u + k^2 u = 0 \quad \text{in} \quad \mathbb{R}^n\backslash\Omega_f$$

and $\qquad u - u^i$ satisfies the radiation condition.

This gives

$$\Delta\delta u + k^2\delta u = 0 \quad \text{in} \quad \mathbb{R}^n\backslash\Omega_f$$

and $\qquad \delta u$ satisfies the radiation condition.

It just remains to find the boundary condition satisfied by δu on $\partial\Omega$. We have

$$u(f(\theta),\theta) = 0 \quad , \quad \theta \in [0,2\pi] \quad .$$

So that

$$(u+\delta u)(f+\delta f(\theta),\theta) = 0 \quad .$$

Now

$$(u+\delta u)(f(\theta) + \delta f(\theta),\theta) = (u+\delta u)(f(\theta),\theta) + \frac{\partial}{\partial r}(u+\delta u)(f(\theta),\theta)\delta f$$
$$+ \text{ second order term in } \delta f$$

from Taylor's theorem.

Combining the two equations gives

$$(u + \delta u)|_{\Omega_f} + \frac{\partial}{\partial r}(u + \delta u)|_{\Omega_f}\,\delta f = 0$$

up to second order terms in δf. As $u|_{\Omega_f} = 0$ and δu is first order in δf (due to the continuity of the map $f \rightarrow u$) we obtain

$$\delta u_{\Omega_f} = -\frac{\partial}{\partial r} u|_{\Omega_f} \delta f$$

up to second order terms.

It follows the Fréchet differential, of the field, $u'(f)s$ is the solution of

$$\begin{aligned} &\Delta u'(f)s + k^2 u'(f)s = 0 \quad \text{in } \mathbb{R}^n \backslash \Omega_f \\ &u'(f)s = -\frac{\partial}{\partial r} u(f) \quad \text{on } \partial\Omega_f \end{aligned} \tag{4.19}$$

and $u'(f)s$ satisfies the radiation condition.

This derivation is somewhat intuitive. However we have also obtained the same equation with the use of separated variable solutions.

Now consider the more general situation in $\mathbb{R}^2$ or $\mathbb{R}^3$ where the starlike scatterer is described by $\underset{\sim}{x} = f(\hat{\underset{\sim}{x}})\hat{\underset{\sim}{x}}$ (see §8.3). Then the boundary condition satisfied by the Fréchet differential can be written

$$u'(f)s = -\hat{\underset{\sim}{x}} \cdot \nabla_x u(f(\hat{\underset{\sim}{x}})\hat{\underset{\sim}{x}})\, s(\hat{\underset{\sim}{x}}) \ , \ \hat{\underset{\sim}{x}} \in \Gamma_o \ . \tag{4.20}$$

This again follows from a Taylor expansion.

From the partial differential equation satisfied by the Fréchet differential it is possible to get an explicit expression for this derivative. We require the Green function $G(f;\underset{\sim}{x},\underset{\sim}{y})$ to satisfy a Dirichlet boundary condition on $\partial\Omega_f$ i.e. $\partial\Omega$ given by $r = f(\theta)$. That is

$$\begin{aligned} &\Delta G(f;\underset{\sim}{x},\underset{\sim}{y}) + k^2 G(f;\underset{\sim}{x},\underset{\sim}{y}) = \delta(\underset{\sim}{y}-\underset{\sim}{x}) \\ &G(f;\underset{\sim}{x},\underset{\sim}{y}) = 0 \ , \ \underset{\sim}{y} \in \partial\Omega_f \end{aligned}$$

and $G(f;\underset{\sim}{x},\underset{\sim}{y})$ satisfies the radiation condition.

Then from the integral representation of the solution (Colton and Kress [1983] p.206) and the boundary condition (4.20)

$$u'(f)s = -\int_{\Gamma_0} \frac{\partial G}{\partial n_y}(f;\underset{\sim}{x},f(\hat{\underset{\sim}{y}})\hat{\underset{\sim}{y}}) \left[\hat{\underset{\sim}{y}} \cdot \nabla_y u(f;f(\hat{\underset{\sim}{y}})\hat{\underset{\sim}{y}})\right] J_f(\hat{\underset{\sim}{y}})\, s(\hat{\underset{\sim}{y}})\, d\hat{\underset{\sim}{y}} \,,$$
$$\underset{\sim}{x} \in \mathbb{R}^n \backslash \Omega_f \quad . \qquad (4.21)$$

Here J_f is the Jacobian of the transformation.

So assuming we measure the solution on some surface M outside Ω (denote these by $U(\underset{\sim}{x})$) then the Newton-Kantorovich method is as follows :

$$f^{(k+1)} = f^{(k)} + s^{(k)}$$

where $s^{(k)}$ solves

$$-\int_{\Gamma_0} \frac{\partial G}{\partial n_y}(f^{(k)};\, \underset{\sim}{x},\, f^{(k)}(\hat{\underset{\sim}{y}})\hat{\underset{\sim}{y}}) \left[\hat{\underset{\sim}{y}} \cdot \nabla_y u(f^{(k)};f^{(k)}(\hat{\underset{\sim}{y}})\hat{\underset{\sim}{y}})\right] s^{(k)}(\hat{\underset{\sim}{y}})\, d\hat{\underset{\sim}{y}}$$
$$= U(\underset{\sim}{x}) - u(f^{(k)};\underset{\sim}{x})\,, \quad \underset{\sim}{x} \in M \quad . \qquad (4.22)$$

This approach would require the additional computation of the Green's function at each iteration. Depending on the particular problem it may still be computationally preferable to use the expression for the Fréchet derivative obtained from the direct problem formulation. The expression is then implicitly defined rather than given by an explicit formula as in (4.21). Also the solution of a 2 x 2 system of operator equations for $s^{(k)}$ and an intermediate quantity (such as $u'(f^{(k)})s^{(k)}$) is required. However, as was seen with the null field method, the additional computation involved is not that much extra.

The explicit expression (4.21) would be very useful in determining either a small perturbation of the boundary from a circle or, if the modified form of the Newton-Kantorovich method was used, starting with a circular approximation to the boundary. Then the required Fréchet derivative could be determined analytically. Later we shall derive the Fréchet derivative of the far field pattern. This is found to be very simple and does not involve a Green's function.

4.5.2 *Hadamard Variation*

The Fréchet derivative (4.21) is closely related to a quantity known as the Hadamard variation. Garabedian [1964] pp.558 studies this for the corresponding potential problem ($k = 0$). The Hadamard variation gives the change in the field due to shifting the boundary $\partial\Omega$ an infinitesimal distance $\delta n(s)$ along its inner normal n (where s is the arc length on $\partial\Omega$).

Then for the potential problem ($k = 0$) and the change in its Green's function, Garabedian obtains

$$\delta G(\underset{\sim}{x},\underset{\sim}{x}') = \int_{\partial\Omega} \frac{\partial G}{\partial n}(\underset{\sim}{y},\underset{\sim}{x}) \frac{\partial G}{\partial n}(\underset{\sim}{y},\underset{\sim}{x}')\, \delta n \, ds \ . \tag{4.23}$$

We can derive such formulas using our variational approach. In this case we have a shift δn in the normal direct, $\hat{\underset{\sim}{n}}$, rather than a shift δf in the radial direction. Now

$$u(\underset{\sim}{x} + \delta n\, \hat{\underset{\sim}{n}}) - u(\underset{\sim}{x}) = \frac{\partial u}{\partial n} \delta n$$

giving

$$\delta u = - \frac{\partial u}{\partial n} \delta n \ \text{ on } \ \partial\Omega \tag{4.24}$$

and δu still satisfies the Helmholtz equation and radiation condition. This results in the variational formula

$$\delta u(\underset{\sim}{x}) = -\int_{\partial\Omega} \frac{\partial}{\partial n} G(\underset{\sim}{y},\underset{\sim}{x}) \frac{\partial u}{\partial n}(\underset{\sim}{y})\, \delta n\, ds \quad . \tag{4.25}$$

An even simpler expression may be derived for the variation of the farfield. The behaviour of the scattered field at infinity in $\mathbb{R}^3$ is given by

$$u^s(\underset{\sim}{x}) = \frac{e^{ik|\underset{\sim}{x}|}}{|\underset{\sim}{x}|} F(\hat{\underset{\sim}{x}}) + O\left[\frac{1}{|\underset{\sim}{x}|^2}\right] \tag{4.26}$$

where $\hat{\underset{\sim}{x}} = \frac{\underset{\sim}{x}}{|\underset{\sim}{x}|}$ and $F(\hat{\underset{\sim}{x}})$ is the far-field pattern.

If $u^s = g$ on $\partial\Omega$ then from the integral representation of the scattered field and the asymptotic behaviour of the Green's function (see Colton and Kress [1983] p.207)

$$F(\hat{\underset{\sim}{x}}) = \int_{\partial\Omega} g(\underset{\sim}{y}) \frac{\partial}{\partial n(\underset{\sim}{y})} u(-\hat{\underset{\sim}{x}};\underset{\sim}{y})\, ds(\underset{\sim}{y}) \quad . \tag{4.27}$$

Here $u(\hat{\underset{\sim}{x}};\underset{\sim}{y})$ is the field resulting from scattering of an incident plane wave $\exp(ik\hat{\underset{\sim}{x}}\cdot y)$ with $u(\hat{\underset{\sim}{x}};\underset{\sim}{y}) = 0$ on $\partial\Omega$.

It follows from (4.24) the Hadamard variation of the farfield is given by

$$\delta F(\hat{\underset{\sim}{x}}) = -\int_{\partial\Omega} \frac{\partial}{\partial n} u(\underset{\sim}{y}) \frac{\partial}{\partial n} u(-\hat{\underset{\sim}{x}};\underset{\sim}{y})\, \delta n\, ds \quad . \tag{4.28}$$

A similar expression holds for the Fréchet derivative of the farfield.

When the field results from the scattering of an incident plane wave $\exp(ik\hat{\underset{\sim}{y}}\cdot y)$ the formula for the Hadamard variation becomes

$$\delta F(\hat{\underset{\sim}{x}},\hat{\underset{\sim}{y}}) = -\int_{\partial\Omega} \frac{\partial}{\partial n} u(-\hat{\underset{\sim}{x}};\underset{\sim}{y}) \frac{\partial}{\partial n} u(\hat{\underset{\sim}{y}};\underset{\sim}{y})\, \delta n\, ds \quad .$$

Here $F(\hat{\underline{x}},\hat{\underline{y}})$ is the far-field in the direction $\hat{\underline{x}}$ resulting from the plane wave given by the direction $\hat{\underline{y}}$.

These expressions are relatively straightforward to use as they only involve the field and no Green function. We note the similarity in form with the Hadamard variation of the total scattering cross-section (4.9) and also the Fréchet derivative of the far-field resulting from refractive index scattering (see Chapter Six).

Several authors have used measurements of the total scattering cross-section to perform reconstructions, because of the straightforward nature of the formula for the Hadamard variation/Fréchet derivative. However, we have here just a simple formula for the Fréchet derivative of the farfield itself. The Newton-Kantorovich method can then easily be derived in a similar manner to (4.22) when field measurements are used.

4.5.3 *A Linear Problem*

Suppose we wish to determine a boundary which is given by a small shift $\delta n(s)$ on a known boundary Ω from farfield measurements. The problem is then linear and described by (4.28) with δn unknown. Assuming data is available for a number of different incident directions $\{\hat{\underline{y}}_j\}_{i=1}^{N}$ and observation angles $\{\hat{\underline{x}}_i\}_{i=1}^{M}$ this then gives a linear moment problem to solve for $\delta n(s)$

$$\delta F(\hat{\underline{x}}_i,\hat{\underline{y}}_j) = - \int_{\partial\Omega} \frac{\partial}{\partial n} u(-\hat{\underline{x}}_i;\underline{y}) \frac{\partial}{\partial n} u(\hat{\underline{y}}_j;\underline{y}) \delta n(s)\, ds\,, \qquad i=1,\ldots,M;\ j=1,\ldots,N\ . \tag{4.29}$$

The solution of such a moment problem is an improperly posed problem. In order to apply regularization methods to its solution we may restrict the solution to a compact set. A suitable choice is to require δn to belong to

$$V = \{\delta n \in C(\partial\Omega): |\delta n(s)| \leq \epsilon, |\delta n(s_1)-\delta n(s_2)| \leq M|s_1-s_2|\} \tag{4.30}$$

where ϵ and M are fixed constants.

Then by the Azéla-Ascoli theorem V is compact in $C(\partial\Omega)$. The Tikhonov selection method could then be applied to regularize the problem. Under these conditions the Backus-Gilbert [1970] method (which Colton and Kirsch [1981a] suggest for the corresponding problem with measurements of the total scattering cross-section) is also applicable.

It should be noted the constraints necessary to regularize this linearized inverse problem are not as strong as those required for the full nonlinear problem. This is typical for many inverse problems, where the linearized map is given by an integral operator but the nonlinear map is given implicitly by a partial differential equation, and so requiring more smoothness on the functions involved.

4.6 IMPEDANCE PROBLEM

In this section we consider the inverse problem of determining the surface impedance of an obstacle Ω of known shape, from a knowledge of the far-field pattern.

The direct problem for the total field u in $\mathbb{R}^2$ is

$$\begin{aligned} &u = u^i + u^s \\ &\Delta u + k^2 u = 0 \quad \text{in} \quad \mathbb{R}^2 \setminus \overline{\Omega} \\ &\frac{\partial u}{\partial n} + \lambda u = 0 \quad \text{on} \quad \partial\Omega \\ &\frac{\partial}{\partial|\underline{x}|} u^s - iku^s \sim o(|\underline{x}|)^{-\frac{1}{2}}, \text{ as } |\underline{x}| \to \infty . \end{aligned} \tag{4.31}$$

The wave number k is positive and fixed, the impedance $\lambda(\underline{x})$ satisfies Im $\lambda \geq 0$, and the scattering obstacle Ω is bounded, connected and has C^2 boundary $\partial\Omega$.

The scattered field has the asymtotic behaviour

$$u^s(\underline{x}) = \frac{1}{4} e^{i(kr+\pi/4)} \sqrt{\frac{2}{\pi kr}} F(\theta;k) + O(r^{-3/2}) \ .$$

Colton and Kress [1983] (Theorem 6.3) show that the impedance $\lambda(\underline{x})$ is uniquely determined by a knowledge of F for a fixed wave number $k > 0$. The proof utilizes Holmgren's Uniqueness Theorem.

This inverse problem is nonlinear - the farfield does not depend linearly upon the impedance. However, Colton and Kirsch [1981b] use a Green function to reduce this nonlinear problem to that of solving two *linear* moment problems where the kernel of the second depends upon the solution of the first.

This approach of Colton and Kirsch requires knowledge of both the amplitude and phase of the farfied at a number of angles from a single incident wave. Their method would not be applicable however if only the amplitude (and not the phase) was known, or if the measurements were taken in one direction at different frequencies etc. Then an iterative method of solution such as the Newton-Kantorovich method is required. This scheme is applicable with measurements of any functional on the field or farfield.

4.6.1 *Continuous Dependence*

We shall show that the farfield pattern depends continuously upon the impedance. The presentation has some things in common with that of Colton and Kirsch [1981b], who prove a similar continuity result. However, we make use of the implicit function theorem, as for the other problems of this thesis. In addition, the stronger result of Fréchet differentiability is obtained.

The differential equation (4.31) is first formulated as an integral equation. We look for a solution u^s in the form

$$u^s(\underset{\sim}{x}) = \frac{i}{4}\int_{\partial D} H_0^{(1)}(k|\underset{\sim}{x} - \underset{\sim}{y}|)\ \phi(\underset{\sim}{y})ds(\underset{\sim}{y})$$

where $H_0^{(1)}$ denotes a Hankel function of the first kind and ϕ is a continuous density to be determined.

The function ϕ then satisfies the following integral equation (see Colton and Kress [1983] p.98)

$$\phi(\underset{\sim}{x}) - \frac{i}{2}\int_{\partial D} \frac{\partial}{\partial n(\underset{\sim}{x})} H_0^{(1)}(k|\underset{\sim}{x}-\underset{\sim}{y}|)\phi(\underset{\sim}{y})ds(\underset{\sim}{y})$$

$$- \lambda(\underset{\sim}{x})\frac{i}{2}\int_{\partial D} H_0^{(1)}(k|\underset{\sim}{x}-\underset{\sim}{y}|)\phi(\underset{\sim}{y})ds(\underset{\sim}{y}) = -2\left[\frac{\partial u^i}{\partial n}(\underset{\sim}{x}) + \lambda(\underset{\sim}{x})u^i(\underset{\sim}{x})\right] \tag{4.32}$$

or

$$\phi - \mathbb{R}\phi - \lambda\mathbb{S}\phi = g_1 + \lambda g_2 \ .$$

Here

$$(\mathbb{R}\phi)(\underset{\sim}{x}) = \frac{i}{2}\int_{\partial D} \frac{\partial}{\partial n(\underset{\sim}{x})} H_0^{(1)}(k|\underset{\sim}{x}-\underset{\sim}{y}|)\phi(\underset{\sim}{y})ds(\underset{\sim}{y}) \ ,$$

$$(\mathbb{S}\phi)(\underset{\sim}{x}) = \int_{\partial D} H_0^{(1)}(k|\underset{\sim}{x}-\underset{\sim}{y}|)\phi(\underset{\sim}{y})ds(\underset{\sim}{y})$$

and $$g_1 = -2\frac{\partial u^i}{\partial n} \ , \quad g_2 = -2u^i \ .$$

We shall assume that the wavenumber k is less than the first eigenvalue, κ_0 of the interior Dirichlet problem for (4.31) in D. Then the integral equation (4.32) is uniquely solvable. This restriction could be removed by considering an integral equation formulation that is uniquely solvable for all wavenumbers.

THEOREM 4.2

If $\lambda,\rho \in C^0(\partial\Omega)$, Im$\lambda \geq 0$ and $k < k_0$ then there exists a unique solution $\phi \in C^0(\partial\Omega)$ of

$$\phi - \mathbb{R}\phi - \lambda \mathbb{S}\phi = \rho \quad .$$

Moreover

$$\|\phi\|_{C^0(\partial\Omega)} \leq \xi \, \|\rho\|_{C^0(\partial\Omega)}$$

for some ξ.

Proof Uniqueness follows as the homogenous form of the equation has nontrivial solutions if and only if the wavenumber k is an interior Dirichlet eigenvalue.

Now from Colton and Kress [1983] p.40 $\mathbb{R}$ and $\mathbb{S}$ are compact operators on $C^0(\partial\Omega)$. The combination $\mathbb{R} + \lambda\mathbb{S}$ is then compact. The existence and boundedness results then follow from the Fredholm alternative theorem. (See the following Chapter - THEOREM 5.1) □

The farfield is given by

$$F(\theta;k) = \int_{\partial D} \phi(y) \exp[-ikr' \cos(\theta-\theta')]ds(y)$$

or

$$F = \mathbb{F}\phi$$

where $\mathbb{F}$: $C(\partial\Omega) \rightarrow C(0,2\pi)$ is compact.

We then have the following continuous dependence result for the maps $\lambda \to \phi(\lambda)$ and $\lambda \to F(\lambda)$.

THEOREM 4.3

If $k < k_0$ and Im $\lambda \geq 0$, then the maps

(i) $\lambda \to \phi(\lambda)$ from $C^0(\partial\Omega) \to C^0(\partial\Omega)$ and

(ii) $\lambda \to F(\lambda)$ from $C^0(\partial\Omega) \to C^0(0,2\pi)$

are both Fréchet differentiable.

<u>Proof</u> (i) We shall apply the implicit function theorem (**THEOREM 1.1**) to (4.32). Set

$$\xi(\lambda,\phi) = \phi - \mathbb{R}\phi - \lambda \mathbb{S}\phi - g_1 - \lambda g_2 \ .$$

Then

$$\xi : C^0(\partial\Omega) \otimes C^0(\partial\Omega) \to C^0(0,2\pi) \ .$$

Checking the conditions of the implicit function theorem

1.
$$\begin{aligned} \delta\xi &= \xi(\lambda + \delta,\phi + \delta\phi) - \xi(\lambda,\phi) \\ &= \delta\phi - \mathbb{R}\delta\phi - \delta\lambda\mathbb{S}\phi - \lambda\mathbb{S}\delta\phi - \delta\lambda\mathbb{S}\delta\phi - \delta\lambda g_2 \end{aligned}$$

giving

$$\begin{aligned} \|\delta\xi\|_{C^0(\partial\Omega)} \leq \|\delta\phi\| &+ \|\mathbb{R}\| \ \|\delta\phi\| \\ &+ \|\mathbb{S}\| \left(\|\phi\| \ \|\delta\lambda\| + \|\lambda\| \ \|\delta\phi\| + \|\delta\lambda\| \ \|\delta\phi\|\right) + \|g_2\| \ \|\delta\lambda\| . \end{aligned}$$

Now $\quad \|\delta\xi\|_{C^0(\partial\Omega)} \to 0 \quad$ as $\quad \|\delta\lambda\|_{C^0(\partial\Omega)}, \|\delta\phi\|_{C^0(\partial\Omega)} \to 0$

so ξ is continuous in λ and ϕ.

2. $\xi_{\phi}(\lambda,\phi)t = t - \mathbb{R}t - \lambda \mathbb{S}t$.

This gives

$$\|\xi_{\phi}(\lambda+\delta\lambda,\ \phi+\delta\phi)t - \xi_{\phi}(\lambda,\phi)t\|_{C^0(\partial\Omega)}$$
$$= \|\delta\lambda \mathbb{S}t\|$$
$$\leq \|\mathbb{S}\|\ \|\delta\lambda\|\ \|t\| .$$

Thus $\xi_{\phi}(\lambda,\phi)$ is continuous in λ and ϕ.

Also

$$\xi_{\lambda}(\lambda,\phi)s = - s\mathbb{S}\phi - sg_2 .$$

This gives

$$\|\xi_{\lambda}(\lambda+\delta,\ \phi+\delta\phi)s - \xi_{\lambda}(\lambda,\phi)s\|_{C^0(\partial\Omega)}$$
$$= \|s\mathbb{S}\delta\phi\|$$
$$\leq \|\mathbb{S}\|\ \|\delta\phi\|\ \|s\| .$$

Hence $\xi_{\lambda}(\lambda,\phi)$ is also continuous in λ and ϕ.

3. $[\xi_{\phi}(\lambda,\phi)]^{-1}$ is bounded from THEOREM 4.2.

The conditions of the implicit function theorem are satisfied and so the map $\lambda \rightarrow \phi(\lambda)$ is Fréchet differentiable.

(ii) $\mathbb{F}$: $C(\partial\Omega) \rightarrow C(0,2\pi)$ is linear and bounded so that the map $\lambda \rightarrow F(\lambda)$ is also Fréchet differentiable. □

The resulting continuity of the map $\lambda \rightarrow F(\lambda)$ may be used to apply regularization techniques to the inverse problem - see Colton and Kirsch [1981b]. They reformulate the problem as a minimization over a compact set resulting from suitable constraints on λ. In the other approach of Colton and Kirsh (where two linear moment problems are solved) an *a priori* bound is required on the gradient of the scattered field on $\partial\Omega$ (the solution of their first moment problem). This is in addition to the constraints on the impedance.

4.6.2 *Generalized Solutions*

We can also consider generalized solutions of this problem. Then we require only $\lambda \in L^{\infty}(\partial\Omega)$ and consider solutions of the integral equation $\phi \in L^2(\partial\Omega)$.

THEOREM 4.4

If $\lambda \in L^{\infty}(\partial\Omega)$, $\rho \in L^{\infty}(\partial\Omega)$, $\mathrm{Im}\,\lambda \geq 0$ and $k < k_0$ then there exists a unique solution $\phi \in L^2(\partial\Omega)$ of

$$\phi - \mathbb{R}\phi - \lambda \mathbb{S}\phi = \rho$$

Moreover

$$||\phi||_{L^2(\partial\Omega)} \leq \xi \; ||\rho||_{L^2(\partial\Omega)}$$

for some ξ.

<u>Proof</u> As Colton and Kress [1983] note, the spectrum is the same as before giving uniqueness for $k < k_0$. The existence and boundedness results then folow from the Fredholm alternative theorem and the compactness of $\mathbb{R}$ and $\mathbb{S}$ on $L^2(\partial\Omega)$. □

Colton and Kress [1983] examine such generalized solutions in the optimal control context where only weak continuity of the map $\lambda \to \phi(\lambda)$ is required. We however can again prove Fréchet differentiability of the map using the implicit function theorem.

THEOREM 4.5

If $k < k_0$ and $\mathrm{Im}\lambda \geq 0$, the map $\lambda \to \phi(\lambda)$ from $L^{\infty}(\partial\Omega) \to L^2(\partial\Omega)$ is Fréchet differentiable.

<u>Proof</u> The steps are analogous to those of the proof of THEOREM 4.3.(i) except that the function spaces involved are suitably changed. Use is made of the regularity result of THEOREM 4.4. □

This result allows for the reconstruction of discontinuous impedances.

4.6.3 *The Fréchet Derivative*

As with the boundary determination problem, there are various ways we could compute the Fréchet derivative for the Newton-Kantorovich method. Firstly, it may be computed from the integral equation (4.32) which gives for the Fréchet differential of the density

$$\phi'(\lambda)s - \mathbb{R}\phi'(\lambda)s - \lambda S\phi'(\lambda)s = s[S\phi + g_2] \quad .$$

Alternatively the Fréchet differential of the impedance to field map $u(\lambda)$, $u'(\lambda)s$ will satisfy the partial differential equation

$$\Delta u'(\lambda)s + k^2 u'(\lambda)s = 0 \quad \text{in } \mathbb{R}^2\backslash\Omega$$

$$\frac{\partial}{\partial n}u'(\lambda)s + \lambda u'(\lambda)s = -u(\lambda)s \quad \text{on } \partial\Omega$$

and

$$\frac{\partial}{\partial|\underline{x}|}u'(\lambda)s - iku'(\lambda)s \sim o(|\underline{x}|^{-\frac{1}{2}}), \text{ as } \underline{x} \to \infty \quad .$$

For the more difficult problem where both the scattering boundary and the impedance are to be determined, clearly an iterative method of solution is also required. Then a combination of the techniques of this section and those of the rest of the chapter would be used to compute the Fréchet derivative and solve the inverse problem. The uniqueness of such an inverse scattering problem is considered in Jones [1985] and Wall [1988b] for the corresponding elastodynamic case.

CHAPTER FIVE

THE MODIFIED HELMHOLTZ EQUATION

5.1 INTRODUCTION

In this chapter we are concerned with scattering by a penetrable object with spatially varying refractive index. In the frequency domain an equation describing this is the modified Helmholtz equation. The corresponding inverse problem is considered in the next chapter. This inverse problem is of particular interest for medical imaging by ultrasound. A closely related inverse problem is the reconstruction of a potential function in the Schrödinger equation for quantum mechanical scattering. Direct and inverse problems for boundary scattering were considered in the previous chapter.

The direct refractive index scattering problem for time-harmonic waves, with time-dependence $\exp(-i\omega t)$ and wave number $k > 0$ is

$$\begin{aligned} \psi(\underline{x}) &= \psi^i(\underline{x}) + \psi^s(\underline{x}), \quad \underline{x} \in \mathbb{R}^n, \; n = 2, 3 \\ \Delta\psi(\underline{x}) &+ k^2 n^2(\underline{x})\,\psi(\underline{x}) = 0, \quad \underline{x} \in \mathbb{R}^n \end{aligned} \tag{5.1}$$

and

$$\frac{\partial\psi^s}{\partial|\underline{x}|} - ik\psi^s \sim o(|\underline{x}|)^{\frac{1-n}{2}}, \text{ as } \underline{x} \to \infty .$$

Here ψ^i is the incident field, ψ^s the scattered field and ψ the total field. These quantities are complex-valued. The last condition of (5.1) is a radiation condition on the scattered field. The index of refraction $n(\underline{x})$ is assumed to be real-valued and unity outside Ω, a region of compact support.

The incident field is produced by sources exterior to Ω, and therefore satisfies the nonhomogeneous equation

$$\Delta\psi^i + k^2\psi^i = f_0(\underset{\sim}{x})$$

where the source term f_0 vanishes in $\overline{\Omega}$. For the case of plane wave incidence

$$\psi^i = e^{i\underset{\sim}{k}.\underset{\sim}{x}} \quad , \quad |\underset{\sim}{k}| = k \ ,$$

the source term $f_0 = 0$ everywhere.

In this chapter some of the properties of the equation (5.1) are outlined. Use shall be made of these later in solving the inverse problem of determining the refractive index from knowledge of the field.

5.1.1 *An Integral Representation*

First consider the case where the refractive index $n = 1$ on the whole of $\mathbb{R}^3$ and a source term, f is present in the equation, that is

$$\nabla\psi + k^2\psi = f \ .$$

Then we have the following integral representation for solutions

$$\psi(\underset{\sim}{x}) = \psi^i(\underset{\sim}{x}) - \int_{\mathbb{R}^3} G_0(\underset{\sim}{x},\underset{\sim}{x}')f(\underset{\sim}{x}')dV' \ . \tag{5.2}$$

Here

$$G_0(\underset{\sim}{x},\underset{\sim}{x}') = \frac{e^{ik|\underset{\sim}{x}-\underset{\sim}{x}'|}}{4\pi|\underset{\sim}{x}-\underset{\sim}{x}'|}$$

is the free-space Green function (which also satisfies the radiation condition).

When the refractive index is spatially varying, that is

$$\Delta\psi + k^2n^2\psi = f$$

then the integral representation becomes

$$\psi(\underset{\sim}{x}) = \psi^i(\underset{\sim}{x}) - \int_{\mathbb{R}^3} G(n;\underset{\sim}{x},\underset{\sim}{x}')f(\underset{\sim}{x}')dV' \quad . \tag{5.3}$$

Here $G(n;\underset{\sim}{x},\underset{\sim}{x}')$ is the Green function associated with the refractive index, n and satisfies

$$\Delta G(n;\underset{\sim}{x},\underset{\sim}{x}') + k^2n^2(\underset{\sim}{x})G(n;\underset{\sim}{x},\underset{\sim}{x}') = \delta(\underset{\sim}{x}-\underset{\sim}{x}')$$

along with the radiation condition.

The integral representation for the free-space problem is used in the next section to derive an equivalent integral formulation of the modified Helmholtz equation. The integral representation for a spatially varying refractive index is used in the next chapter on the inverse problem to derive the Fréchet derivative of the refractive index to field map.

5.1.2 *Existence and Uniqueness*

An existence and uniqueness result for the equation (5.1) has been proven in Leis [1967] (see also Weston [1980]). This states if n(x) is real and continuous, with D a compact domain containing Ω, then there exists a unique solution to the direct scattering problem $\psi\epsilon C^2(\overline{D})$, provided that the incident wave ψ^i is continuous in D (i.e. all sources external to D). Use is made of the unique continuation principle (Leis [1986]).

Colton and Monk [1988] also considered an equivalent integral equatio formulation, obtaining existence and uniqueness for continuously differentiabl refractive index and field, $\psi \in L^2(D)$. Uniqueness was obtained using the uniqu continuation theorem from Müller [1969] Chapter Six. Müller also prove existence and uniqueness for continuous solutions of Maxwell's equations wit spatially varying coefficient functions. A similar uniqueness (but not existence result is given by Jones [1982] for an elastodynamic problem - this makes extensiv use of the properties of spherical harmonics.

A uniqueness result for solutions of the modified Helmholtz equation i proven in Wall [1988a] for piecewise analytic refractive indicies. These results are used later in the chapter along with the Fredholm alternative theorem to prove the existence and regularity of solutions in the Sobolev space, $H^2(D)$.

To show the uniqueness result, Wall uses an approach generalizing that of Kress and Roach [1978]. These last authors prove uniqueness for piecewise homogenous bodies. They then formulated the problem as a system of boundary integral equations and prove an existence result using Fredholm theory - see also Colton and Kress [1983]. Uniqueness results for piecewise homogenous nested bodies for the corresponding elastodynamic problem have been proven in Kupradze [1979] (and also Jones [1982]).

Volume integral equation methods for this problem with spatially varying refractive index, but with also a transmission condition on the boundary $\partial\Omega$ are examined in Wall [1988c,d] (see also Kleinmann and Martin [1987]). Existence and uniqueness results are obtained for such equations using both first and second kind integral equation methods.

The key to proving uniqueness with minimum regularity requirements on the coefficient of the partial differential equation is the use of the unique continuation principle (Leis [1986], Hörmander [1983]). This principle states that if ψ is a solution of an elliptic equation in a doman D and it vanishes in a neighbourhood of a point $\underline{x}_0 \in D$, then it vanishes identically in D. For the case when the coefficients of the differential equation are analytic the principle is clear, what is remarkable is that it is also valid for the case with non-analytic coefficients.

We now state the Fredholm alternative theorem which is a keystone in the theory of existence and regularity for linear partial differential and integral equations. The net result of this theorem is that uniqueness is equivalent to existence of a solution. The theorem was used for some of the existence results just described. It will be utilized later to prove further existence and regularity results for the Helmholtz equation.

THEOREM 5.1

Assume
$$(\lambda I - T)f = g$$

where $\lambda \in \mathbb{C}$ with $\lambda \neq 0$ and $T : X \to X$ is a compact linear operator with X a Banach space.

Then uniqueness of a solution to this equation implies

(i) Existence of a solution.

(ii) $(\lambda I - T)^{-1}$ is bounded with

$$f = (\lambda I - T)^{-1} g .$$

<u>Proof</u> See Hutson and Pym [1980] for example. □

In the remainder of this chapter we consider in more detail three particular existence and uniqueness theories for the modified Helmholtz equation. Firstly, the equation is reformulated as an equivalent integral equation. Then Fredholm theory is applied in the space of continuously differentiable functions. Next, the solution of this integral equation via Neumann series is investigated. Finally, the existence of the solution of the Helmholtz equation in the Sobolev space H^2 is attempted.

In the last section of the chapter we outline possible numerical schemes fo the solution of the Helmholtz equation with spatially varying refractive index.

5.2 AN INTEGRAL EQUATION

Assuming plane wave incidence, then the modified Helmholtz equation may be formulated in the equivalent form (see Colton [1980] p.39)

$$\psi(\underline{x}) = \psi^i(\underline{x}) + k^2 \int_\Omega G_0(\underline{x},\underline{x}')[n^2(\underline{x}') - 1]\psi(\underline{x}')dV' \ , \ \underline{x}\epsilon\mathbb{R}^3 \tag{5.4}$$

where

$$G_0(\underline{x},\underline{x}') = \frac{e^{ik|\underline{x}-\underline{x}'|}}{4\pi|\underline{x}-\underline{x}'|}$$

again is the free-space Green function for the Helmholtz equation in three-dimensional space. We require $\partial\Omega$ to be smooth enough for Green's theorems to be applicable (see §2.2.1).

The equation remains valid for $\underline{x} \epsilon D$, where D is a compact domain in $\mathbb{R}^3$, if all sources are external to D (i.e. $f_0(\underline{x}) = 0$, $\underline{x} \epsilon D$).

To see how this equation is derived the modified Helmholtz equation (5.1) is rewritten as

$$\Delta\psi + k^2\psi + k^2(n^2-1)\psi = 0 \ .$$

But

$$\psi = \psi^i + \psi^s \quad \text{and} \quad \Delta\psi^i + k^2\psi^i = 0 \ \text{in D}$$

so

$$\Delta\psi_s + k^2\psi_s = -(n^2-1)\psi, \ \ \underline{x} \epsilon D \ .$$

Using the integral representation (5.2) the following is obtained

$$\psi_S(\underline{x}) = k^2 \int_\Omega G_0(\underline{x},\underline{x}')[n^2(\underline{x}')-1]\psi(\underline{x}')dV' \ , \ \underline{x} \in D$$

as required.

The Green function $G(n;\underline{x},\underline{x}')$ satisfies a similar integral equation to (5.4). From Weston [1980] the Green function has the decomposition

$$G(n;\underline{x},\underline{x}') = G_0(\underline{x},\underline{x}') + \tilde{G}(n;\underline{x},\underline{x}') \ .$$

$\tilde{G}(n;\underline{x},\underline{x}')$ is a continuous function of $\underline{x}$ and $\underline{x}'$ satisfying the integral equation

$$\begin{aligned}\tilde{G}(n;\underline{x},\underline{x}') = {} & k^2 \int_\Omega G_0(\underline{x},\underline{x}'')\, G_0(\underline{x}'',\underline{x}')[n^2(\underline{x}'') - 1]dV'' \\ & + k^2 \int_\Omega G_0(\underline{x},\underline{x}'')\, \tilde{G}(n;\underline{x}'',\underline{x}')[n^2(\underline{x}'') - 1]dV'' .\end{aligned} \tag{5.5}$$

5.2.1 *Weakly Singular Integral Operators*

Before we obtain existence and regularity results for the integral equation (5.4) the mapping properties of weakly singular integral operators are examined.

Let Ω and D be bounded sets in n-dimensional Euclidean space, and $A(\underline{x},\underline{x}')$ a continuous function bounded on Ω x D

$$|A(\underline{x},\underline{x}')| \leq C = \text{const.}$$

The function

$$k(\underline{x},\underline{x}') = \frac{A(\underline{x},\underline{x}')}{|\underline{x}-\underline{x}'|^\alpha} \ , \quad \alpha < n$$

of the points $\underset{\sim}{x},\underset{\sim}{x}'$, is called a kernel with a weak singularity. The operator K defined by the formula

$$(Ku)(\underset{\sim}{x}) = \int_{\Omega} k(\underset{\sim}{x},\underset{\sim}{x}')u(\underset{\sim}{x}')dV'$$

$$= \int_{\Omega} \frac{A(\underset{\sim}{x},\underset{\sim}{x}')}{|\underset{\sim}{x}-\underset{\sim}{x}'|^{\alpha}} u(\underset{\sim}{x}')dV' \tag{5.6}$$

is called an integral operator with a weak singularity - see Miklin [1970] p.158.

LEMMA 5.1

The integral operator with a weak singularity (5.6) is bounded

(i) from the space $C^0(\overline{\Omega})$ into $C^0(\overline{D})$,

(ii) from the space $L^2(\Omega)$ into $C^0(\overline{D})$,

if $\alpha \leq \frac{n}{2}$.

<u>Proof</u> (i) See Miklin [1970] p.162 :

$$|(Ku)(\underset{\sim}{x})| \leq \left| \int_{\Omega} \frac{A(\underset{\sim}{x},\underset{\sim}{x}')}{|\underset{\sim}{x}-\underset{\sim}{x}'|^{\alpha}} u(\underset{\sim}{x}')dV' \right|$$

$$\leq C\left[\int_{\Omega} \frac{dV'}{|\underset{\sim}{x}-\underset{\sim}{x}'|^{\alpha}}\right]||u||_{\infty,\Omega}$$

The integral is bounded for $\alpha < n$ and so K is bounded.

<u>Proof</u> (ii) $$|(Ku)(\underline{x})| \leq \left| \int_\Omega \frac{A(\underline{x},\underline{x}')}{|\underline{x}-\underline{x}'|^\alpha} u(\underline{x}')dV' \right|$$

$$\leq C \int_\Omega \left| \frac{1}{|\underline{x}-\underline{x}'|^\alpha} u(\underline{x}') \right| dV'$$

$$\leq C \left[\int_\Omega \frac{dV'}{|\underline{x}-\underline{x}'|^{2\alpha}} \right] ||u||_{2,\Omega}$$

using the Schwartz inequality.

The integral is bounded for $2\alpha < n$ and so K is bounded. □

5.2.2 *Regularity*

We shall require $n \epsilon C^0(\overline{\Omega})$ and consider ψ^i and $\psi \epsilon C^1(\overline{D})$. Setting $\nu = n^2$ we have the following operator forms for the integral equation (5.4)

$$\psi = \psi^i + \overline{K}(\nu-1)\psi\,, \tag{5.7}$$

where $$\overline{K} = k^2 \int_\Omega G_0 \quad \text{and} \quad \overline{K} : C^0(\overline{\Omega}) \to C^1(\overline{D})$$

or

$$\psi = \psi^i + \overline{K}_\nu \psi\,, \tag{5.8}$$

where

$$\overline{K}_\nu = \overline{K}(\nu-1) \quad \text{and} \quad \overline{K}_\nu : C^1(\overline{D}) \to C^1(\overline{D})\ .$$

The boundedness of the operators $\overline{K}$ and $\overline{K}_\nu$ follows as they are both weakly singular integral operators.

LEMMA 5.2 With $\nu \in C^0(\overline{\Omega})$ both

(i) $\overline{K} : C^0(\overline{\Omega}) \to C^1(\overline{D})$ and

(ii) $\overline{K}_\nu : C^1(\overline{D}) \to C^1(\overline{D})$

are bounded linear operators.

Proof (i) The kernel of $\overline{K}$ is

$$G_0(\underset{\sim}{x},\underset{\sim}{x}') = \frac{1}{4\pi} \frac{e^{ik|\underset{\sim}{x}-\underset{\sim}{x}'|}}{|\underset{\sim}{x} - \underset{\sim}{x}'|} ,$$

which is weakly singular with $\alpha = 1$ (and $C = \frac{1}{4}\pi$). As $n = 3$, it follows $\overline{K} : C^0(\overline{\Omega}) \to C^0(\overline{D})$ is bounded.

For boundedness into $C^1(\overline{D})$ we examine by taking the gradient

$$\nabla(\overline{K}u)(\underset{\sim}{x}) = \int_\Omega \nabla G_0(\underset{\sim}{x},\underset{\sim}{x}')\, u(\underset{\sim}{x}')dV' .$$

Now the kernel still contains a weak singularity, but with $\alpha = 2$. However, $\alpha < n$ still, so that $\overline{K} : C^0(\overline{\Omega}) \to C^1(\overline{D})$ is bounded as required.

(ii) $$(\overline{K}_\nu u)(\underset{\sim}{x}) = \int_\Omega G_0(x,\underset{\sim}{x}')[\nu(\underset{\sim}{x}') - 1]\, u(\underset{\sim}{x}')dV'$$

and

$$\nabla(\overline{K}_\nu u)(\underset{\sim}{x}) = \int_\Omega \nabla G_0(\underset{\sim}{x},\underset{\sim}{x}')[\nu(\underset{\sim}{x}') - 1]\, u(\underset{\sim}{x})dV' .$$

As $\nu(\underset{\sim}{x}')$ is continuous, like $\overline{K}$, $\overline{K}_\nu : C^0(\overline{D}) \to C^1(\overline{D})$ is bounded. Hence also $\overline{K}_\nu : C^1(\overline{D}) \to C^1(\overline{D})$ is bounded as required. □

Given a uniqueness result for this equation we can use the Fredholm alternative to prove the existence of a solution and also a boundedness result.

This result will be proven for the solution on some compact domain D which encloses Ω and then the field belongs to the Banach space $C^1(\overline{D})$.

We note that Leis [1967] proved existence and uniqueness in $C^2(\overline{D})$. This utilized the unique continuation principle and a principle of limiting absorption, i.e. $\lim_{k_c \to 0} (k_r + ik_c) = k_r$ (see also Leis [1986]).

Also we require a result bounding the solution in terms of a source term in the integral equation. This is used in the next chapter to prove the Fréchet differentiability of the refractive index to field map via the implicit function theorem.

We obtain the existence of a solution in $C^1(\overline{D})$ rather than $C^2(\overline{D})$ as the integral operator $\overline{K}$ with a weak singularity only maps $C^0(\overline{\Omega})$ into $C^1(\overline{D})$ and not $C^2(\overline{D})$. [See the proof of Lemma 5.2 - this would then require $\alpha = n$. In fact, such an operator as $\overline{K}$ maps from $C^{0,\alpha}$ into C^2, i.e. Hölder continuity is required.]

THEOREM 5.2

If $n \in C^0(\overline{\Omega})$ and $\psi^i \in C^1(\overline{D})$ then there exists a unique solution $\psi \in C^1(\overline{D})$ of (5.4). Moreover

$$||\psi_{C^1(\overline{D})}|| \leq \zeta ||\psi^i||_{C^1(\overline{D})}$$

for some constant ζ.

<u>Proof</u> See Weston [1984] for the required uniqueness result - the work of Leis [1967] is used in obtaining it. The existence and boundedness results then follow from the Fredholm alternative theorem (THEOREM 5.1) applied to

$$(I - \overline{K}_\nu)\, \psi = \psi^i \ .$$

For this the compactness of $\overline{K}_\nu : C^1(\overline{D}) \to C^1(\overline{D})$ is required. As $\overline{K}_\nu$ is an integral operator with a weak singularity with $\alpha = 1$, from the proof of LEMMA 5.2 (ii) $K_\nu : C^0(\overline{D}) \to C^1(\overline{D})$ is bounded. Now the imbedding $C^1(\overline{D}) \to C^0(\overline{D})$ is compact - from Adams [1975] p.11. The composition of a compact operator and a bounded operator is compact giving the desired result. □

Weston claims the Leis uniqueness result extends to a class of piecewise continuous refractive indicies but does not indicate how. The quantities ψ and $\frac{\partial \psi}{\partial n}$ are required to be continuous across discontinuity boundaries so that ψ is still C^1. If this uniqueness result is valid, then THEOREM 5.2 also gives an existence and regularity result for such piecewise continuous refractive indicies. The proof changes slightly in that the integral over the region Ω is broken up into a sum of integrals over the various regions on which n is continuous.

5.3 BORN SERIES

One method for solving the integral equation (5.4) is by iteration or Neumann series. The resulting series for this problem is known as the Born series and its truncation after one term as the Born approximation. As will be shown, this approach converges when the frequency is low enough and the refractive index does not vary too far from unity (in the L^2 norm).

For numerical computation the approach taken is to compute ψ inside Ω using the series. Then ψ is calculated outside using the right-hand side of the integral equation (5.4). In two-dimensions some actual computations have been performed by Johnson and Tracy [1985] in the process of solving the inverse problem.

The integral equation may be written as

$$\psi = \psi^{i} + K(\nu\text{-}1)\psi \quad \text{where} \quad K = k^2\int_{\Omega} G_0 \tag{5.10}$$

where

$$\nu = n^2 \quad ,$$

or alternatively

$$\psi = \psi^{i} + K_{\nu}\psi \quad \text{where} \quad K_{\nu} = K(\nu\text{-}1) \ . \tag{5.11}$$

We shall require ν - 1 ϵ $L^2(\Omega)$ and ψ ϵ $C^0(\overline{\Omega})$ so that K: $L^2(\Omega) \rightarrow C^0(\overline{\Omega})$ and K_{ν}:$C^0(\overline{\Omega}) \rightarrow C^0(\overline{\Omega})$. The boundedness of the operator K follows as it is an integral operator with weakly singular kernel.

LEMMA 5.3 With ν ϵ $L^2(\Omega)$ both

(i) K : $L^2(\Omega) \rightarrow C^0(\overline{D})$ and (ii) K_{ν}:$C^0(\overline{D}) \rightarrow C^0(\overline{D})$ are bounded linear operators.

Proof (i) Follows from Lemma 5.1 (ii), as the kernel of K is weakly singular with $\alpha = 1 < \frac{n}{2}$.

(ii) We have

$$\begin{aligned} ||K_{\nu}u||_{C^0(\overline{D})} &= ||K(\nu\text{-}1)u||_{C^0(\overline{D})} \\ &\leq ||K||\,||(\nu\text{-}1)u||_{L^2(\Omega)} && \text{[from (i)]} \\ &\leq ||K||\ ||\nu\text{-}1||_{L^2(\Omega)}||u||_{\infty,\Omega} \\ &\leq ||K||\ ||\nu\text{-}1||_{L^2(\Omega)}||u||_{C^0(\overline{D})} \end{aligned}$$

so that

$$||K_{\nu}||_{\infty} \leq ||K||\ ||\nu\text{-}1||_{L^2(\Omega)}$$

and K_{ν}: $C^0(\overline{D}) \rightarrow C^0(\overline{D})$ is bounded. □

5.3.1 *Regularity*

Given the boundedness of the operator K_ν, Banach's theorem may be used to prove existence and uniqueness of solutions to (5.10) and also boundedness of $(I - K_\nu)^{-1}$.

THEOREM 5.3 (Banach's Theorem)

Let A be a bounded, linear operator, acting in a Banach space X, and let $||A|| < \frac{1}{\lambda}$. Then the operator $(I - \lambda A)^{-1}$, where I is the unit operator, exists, it is defined on the whole space X, and is bounded. In addition

$$(I - \lambda A)^{-1} = \sum_{n=0}^{\infty} (\lambda A)^n$$

and

$$||(I - \lambda A)^{-1}|| \leq (1 - ||\lambda A||)^{-1} .$$

<u>Proof</u> By the completeness of $L(X)$ - see Hutson and Pym [1980] p.86 for example. □

THEOREM 5.4 If $||K(\nu\text{-}1)||_\infty = ||K_\nu||_\infty < 1$ then there exists a unique solution $\psi \in C^0(\overline{\Omega})$ to the integral equation (5.4) with

$$\psi = \psi^i + K_\nu \psi^i + K_\nu^2 \psi^i + \;....$$

and

$$||\psi||_{\infty,\Omega} \leq \frac{||\psi^i||_{\infty,\Omega}}{1 - ||K_\nu||_\infty} .$$

<u>Proof</u> Follows from applying Banach's theorem to (5.2) which may be written as

$$(I - K_\nu)\psi = \psi^i .$$

□

COROLLARY 5.1

The error in truncating the series of the Nth iterate is

$$||\psi - \sum_{j=0}^{N} K_\nu^j \psi^i||_{\infty,\Omega} \leq \frac{||K_\nu||_\infty^N \; ||\psi^i||_{\infty,\Omega}}{1 - ||K_\nu||} \; . \qquad \square$$

In particular the error in the first iterate is

$$||\psi - \psi^i - K_\nu \psi^i||_{\infty,\Omega} \leq \frac{||K_\nu||_\infty^2 \; ||\psi^i||_{\infty,\Omega}}{1 - ||K_\nu||} \; .$$

COROLLARY 5.2

If $||K_\nu||_\infty < 1$, then there exists a unique solution $\psi \in C^0(\overline{D})$, where all sources are external to the compact domain D.

Proof The equation (5.4) gives the unique continuation of ψ onto $\overline{D}$ (see Colton [1980] p.39). □

Thus if the condition

$$||K_\nu||_\infty = \sup_\psi \frac{||k^2 \int_\Omega G_0(\underline{x},\underline{x}')[\nu(\underline{x}') - 1]\psi(\underline{x}')dV'||_{\infty,\Omega}}{||\psi||_{\infty,\Omega}} < 1 \qquad (5.12)$$

is satisfied we may solve the direct problem by iteration. The solution outside the region is then given by (5.4).

The Born approximation to the solution is given by the first iterate

$$\psi(\underline{x}) = \psi^i(\underline{x}) + k^2 \int_\Omega G_0(\underline{x},\underline{x})[n^2(\underline{x}') - 1]\psi^i(\underline{x}')dV' \; . \qquad (5.13)$$

The error in the approximation is given by COROLLARY 5.1, and so (5.13) is then a good approximation to the solution if $||K_\nu|| << 1$. We note that (5.13) is what results from approximating the field, ψ, by the incident field, ψ^i inside the integral equation (5.2).

The following theorem from Colton [1980] gives a sufficiency condition for $||K_\nu|| < 1$. Assume Ω is a sphere, i.e. $\Omega = \{\underset{\sim}{x} : |\underset{\sim}{x}| \le a\}$. There is no difficulty if it is not a sphere as then the smallest sphere containing Ω may be considered.

THEOREM 5.5 Let $\mu = \max_{\underset{\sim}{x} \in \Omega} |\nu(\underset{\sim}{x}) - 1|$. Then $||K_\nu|| < 1$ whenever $k^2 < \dfrac{2}{\mu a^2}$.

<u>Proof</u>

$$|(K_\nu\psi)(\underset{\sim}{x})| = \frac{k^2}{4\pi}\left|\int_\Omega \frac{e^{ik|\underset{\sim}{x}-\underset{\sim}{x}'|}}{|\underset{\sim}{x} - \underset{\sim}{x}'|}[\nu(\underset{\sim}{x}')-1]\psi(\underset{\sim}{x}')\right|dV'$$

$$\le \frac{k^2\mu}{4\pi}||\psi||_{\infty,\Omega} \int_\Omega \frac{dV'}{|\underset{\sim}{x} - \underset{\sim}{x}'|} .$$

Now from Colton [1980] p.40

$$\int_\Omega \frac{dV'}{|\underset{\sim}{x} - \underset{\sim}{x}'|} \le 2\pi a^2 .$$

So

$$|(K_\nu\psi)(\underset{\sim}{x})| \le \tfrac{1}{2}k^2\mu a^2||\psi|| ,$$

that is

$$||K_\nu|| \le \tfrac{1}{2}k\mu a^2 .$$

Hence $||K_\nu|| < 1$ whenever $k^2 < \dfrac{2}{\mu a^2}$. □

Note that this result requires a stronger condition on the refractive index than $n^2 - 1 \in L^2(\Omega)$ which was required earlier. For this theorem $\max|n^2 - 1|$ bounded is necessary, i.e. $n^2 \in L^\infty(\Omega)$.

A similar result was obtained by Leeman *et al.* [1985] when considering scattering by a sphere of constant refractive index (not necessarily equal to unity).

We now give a result of our own that only needs ν square integrable. This will also be more useful for our purposes when we consider the inverse problem in the next chapter.

THEOREM 5.6

Let $\mu' = ||\nu - 1||_{L^2(\Omega)}$.
Then $||K_\nu|| < 1$ whenever $k^2 < \dfrac{1}{\mu' a}$.

Proof

$$|(K_\nu\psi)(\underline{x})| = \frac{k^2}{4\pi}\left|\int_\Omega \frac{e^{ik|\underline{x}-\underline{x}'|}}{|\underline{x} - \underline{x}'|}[\nu(x') - 1]\psi(\underline{x}')dV'\right|$$

$$\leq \frac{k^2}{4\pi}||\psi||_{\infty,\Omega} \int_\Omega \left| \frac{1}{|\underline{x} - \underline{x}'|}[\nu(\underline{x}') - 1]\right| dV'$$

$$\leq \frac{k^2\mu'}{4\pi}||\psi||_{\infty,\Omega} \int_\Omega \frac{dV'}{|\underline{x} - \underline{x}'|^2}$$

from using the Schwartz inequality.

Now from Miklin [1970] p.159

$$\int_\Omega \frac{dV'}{|\underline{x} - \underline{x}'|^2} \leq 4\pi a \ .$$

So

$$|(K_\nu\psi)(\underline{x})| \leq k^2\mu' a||\psi|| \ ,$$

that is

$$||K_\nu|| \leq k^2\mu' a \ .$$

Hence $||K_\nu|| < 1$ whenever $k^2 < \frac{1}{\mu' a}$. □

The analogous result for a one-dimensional scattering problem is contained in Bates and Wall [1976].

We note that when the region Ω has a constant refractive index (not necessarily unity) a boundary integral equation may be derived for the field - rather than (5.4) which contains an integral over Ω. Kittapa and Kleinmann [1975] investigate the use of Neumann series to solve this equation. Neumann series methods for boundary scattering problems are considered in Colton and Kress [1983].

5.4 SOBOLEV SPACE THEORY

In Wall [1988a] a uniqueness result for solutions of the modified Helmholtz equation with piecewise analytic refractive indices was shown. As is outlined later, the requirement for uniqueness may be weakened to piecewise C^1 refractive indices.

We shall prove an existence and regularity result for such solutions in a Sobolev space $H^2(D)$, where again D is a compact domain containing Ω. To obtain the existence result we make sure of the Fredholm alternative theorem which in turn requires uniqueness.

The result shall be proved for the equation

$$\Delta\psi(\underline{x}) + k^2 n^2(\underline{x})\psi(\underline{x}) = f(\underline{x}) \ , \ \underline{x} \in \mathbb{R}^3 \tag{5.14}$$

and

$$\frac{\partial \psi}{\partial |\underset{\sim}{x}|} + ik\psi \sim o(|\underset{\sim}{x}|)^{-1} \qquad \text{as} \qquad \underset{\sim}{x} \to \infty \; .$$

with $\mathrm{supp}(n^2 - 1) \subset \Omega$ and $\mathrm{supp}\, f \subset D$.

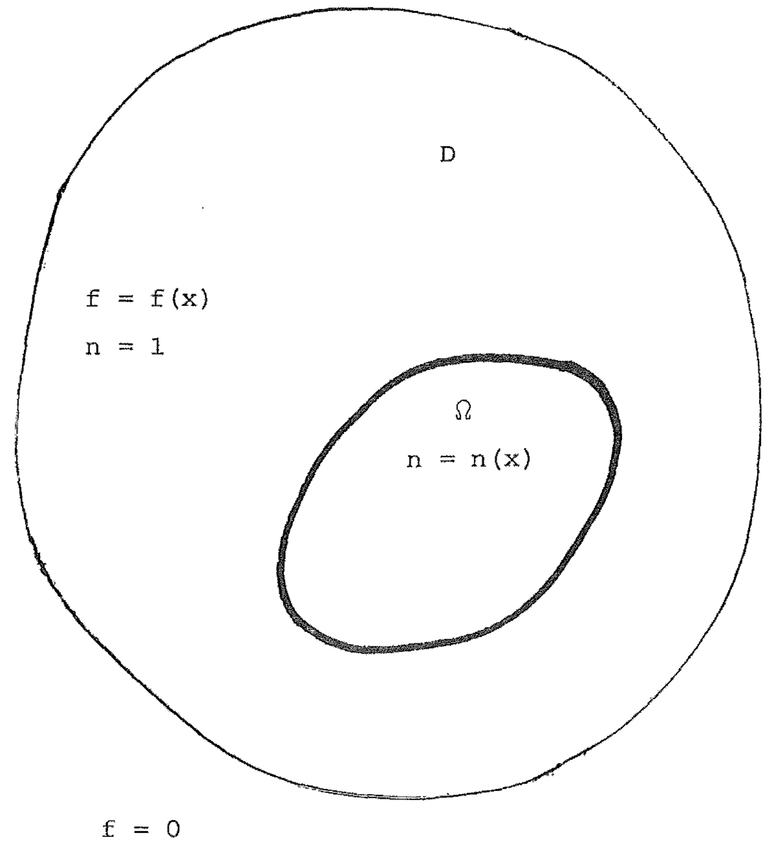

Figure 5.1

Scattering of an incident wave with sources in D is a special case of the equation (5.14). Here we split the wave function into the incident field and the scattered field, which satisfies the radiation condition. That is

$$\Delta\tilde{\psi} + k^2n^2\tilde{\psi} = 0 \qquad , \quad \underline{x} \in \mathbb{R}^3$$

with
$$\tilde{\psi} = \tilde{\psi}^i + \tilde{\psi}^s \qquad , \quad \underline{x} \in \mathbb{R}^3$$

and
$$\frac{\partial\tilde{\psi}^s}{\partial|\underline{x}|} + i\,k\,\tilde{\psi}^s \sim o(|\underline{x}|)^{-1} \quad \text{as} \quad \underline{x} \to \infty \ .$$

This gives
$$\Delta(\tilde{\psi}^i + \tilde{\psi}^s) + k^2n^2(\tilde{\psi}^i + \tilde{\psi}^s) = 0$$

or
$$\Delta\tilde{\psi}^s + k^2n^2\tilde{\psi}^s = -\,\Delta\tilde{\psi}^i - k^2n^2\tilde{\psi}^i \ .$$

But
$$\Delta\tilde{\psi}^i + k^2\tilde{\psi}^i = f_0$$

so that
$$\Delta\tilde{\psi}^s + k^2n^2\tilde{\psi}^s = k^2(1-n^2)\tilde{\psi}^i - f_0 \, , \quad \underline{x} \in \mathbb{R}^3 \ .$$

So setting $\psi = \tilde{\psi}^s$ and $f = k^2(1-n^2)\tilde{\psi}^i - f_0$ we see this is a special case of (5.14) with supp $f \subset \Omega$ as $n = 1$ outside Ω and also supp $f_0 \subset D$. This case also clearly caters for plane wave incidence (then $f_0 = 0$ everywhere).

As the refractive index is required to be piecewise C^1, the existence and uniqueness result will be particularly suitable for the computational setting. Here we must approximate the material parameters of the body by piecewise polynomials.

The regions which have boundaries across which the refractive index is not analytic are defined by a tree-like structure in Wall [1988a] - see Figure 5.2. This allows for subregions with corners and in particular the finite element structure that might occur in a typical computational problem and to which our existence and regularity result is applicable.

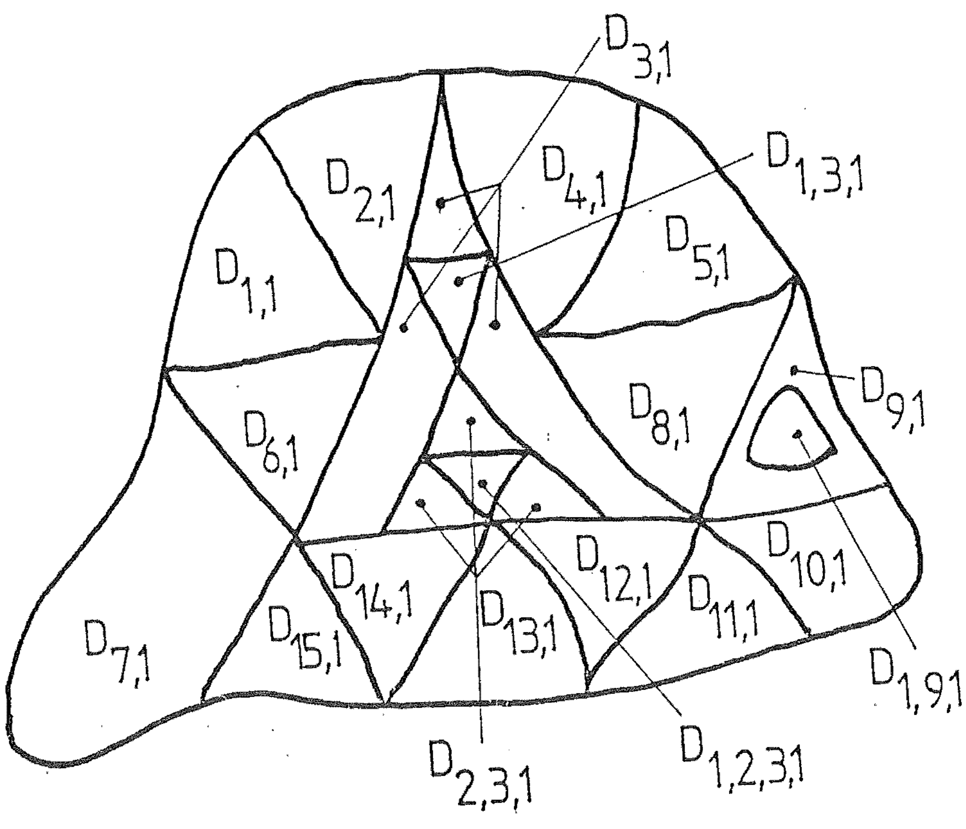

Figure 5.2

5.4.1 *Uniqueness*

We shall assume the refractive index is real. It should be noted Wall [1988a] does obtain uniqueness for complex values of $\nu = n^2$, however with some restrictions. These are necessary as the solution of the problem is not in general unique for arbitrary complex ν. See Kress and Roach [1978] for a piecewise homogeneous case with complex ν exhibiting nonuniqueness.

To prove uniqueness for the equation (5.14) it suffices because the p.d.e. is linear to just consider the homogeneous equation

$$\Delta\psi + k^2n^2\psi = 0 \text{ in } \mathbb{R}^3$$

and
$$\frac{\partial\psi}{\partial|\underline{x}|} + i\,k\,\psi \sim o(|\underline{x}|)^{-1} \;, \text{ as } \underline{x} \to \infty \;.$$

Wall's uniqueness result for this interior-exterior problem revolves about the proof for the interior problem with Cauchy data, i.e. $u = 0$ and $\frac{\partial\psi}{\partial n} = 0$ on $\partial\Omega$. Then when n is analytic the Cauchy-Kovalevskaia theorem asserts the existence of a unique, analytic solution in the neighbourhood of this surface. Also necessary is the Holmgrem extension to this theorem, which assures us that this is the only solution even among non-analytic solutions. In the piecewise analytic case (see the paper for a definition) the zero solution can be continued via the jump conditions across discontinuity boundaries, and so covering the whole region. The Rellich Lemma and analyticity arguments are then used to show uniqueness for the original interior-exterior problem.

However, as was noted earlier, the unique continuation principle is valid for a non-analytic coefficient function. In fact, Müller [1969] and Colton and Monk [1988] have proven uniqueness for solutions of the modified Helmholtz equation with a C^1 refractive index. We then can extend the uniqueness result of Wall [1988a] to real piecewise C^1 indices - see Wall [1988b].

It may be possible to weaken the regularity requirement on the refractive index still further. From Hörmander [1983] a version of the unique continuation principle known as the Aronszajn-Cordes uniqueness theorem is valid for just a bounded coefficient function.

As this problem involves edges and corners (the refractive index is piecewise C^1) to obtain a unique solution to the problem the edge condition

(Jones [1986]) must be satisfied. This requires the energy density to be integrable over any finite region (even if this domain contains singularities of the field). We note that specifying the field to belong to the space $H^2(D)$ automatically imposes this condition on the field.

5.4.2 *Existence and Regularity*

For our existence result we shall require the refractive index to be piecewise C^1. Then the solution of the partial differential equation is unique and also $n \in L^\infty(\Omega)$.

THEOREM 5.7 If n is real and piecewise C^1 with $\mathrm{supp}(n^2-1) \subset \Omega$ and $f \in L^2(D)$, then there exists a unique solution $\psi \in H^2(D)$ of (5.14). Moreover

$$\|\psi\|_{H^2(D)} \le \xi \|f\|_{L^2(D)}$$

for some constant ξ.

Proof Let v be the solution of the free-space outgoing problem

$$\Delta v + k^2 v = g\,, \quad \mathrm{supp}\, g \subset D \text{ with } g \in L^2(D)\,.$$

Then there exists a unique solution for v ,

$$v = R\, g\,.$$

From the integral representation (5.2) for v in terms of g we have (see Phillips [1973] for example)

$$\|v\|_{2,D} \leq C\|g\|_{0,D} \ .$$

That is $R : L^2(D) \to H^2(D)$ is bounded.

Now

$$\Delta\psi + k^2n^2\psi = f \ ,$$

so that

$$\Delta\psi + k^2\psi = f - k^2(n^2 - 1)\psi \ ,$$

and

$$\psi = Rf - k^2R[(n^2 - 1)\psi] \ .$$

Rewrite this as

$$\psi - \tilde{K}\psi = Rf$$

where

$$\tilde{K} = k^2R(1 - n^2) \ .$$

To apply Fredholm theory giving us the existence and boundedness of $(I - \tilde{K})^{-1}$ we need to show

(a) $\tilde{K} : H^2(D) \to H^2(D)$ is compact.

(b) $(I - \tilde{K})$ is one-to-one; i.e. there is a unique solution to $w - \tilde{K}w = 0$ the homogeneous equation.

(a) K is compact

Now

$$R : L^2(D) \to H^2(D) \text{ is bounded.}$$

As $n \in L^{\infty}(\Omega)$ we then have

$$\tilde{K} : L^2(D) \to H^2(D) \text{ is bounded.}$$

But the imbedding $H^2(D) \to L^2(D)$ is compact, and as the composition of a bounded and a compact operator is compact it follows

$$\tilde{K} : H^2(D) \to H^2(D) \text{ is compact.}$$

(b) I-K one-to-one

Suppose $\quad w - \tilde{K}w = 0$

then $\quad w = - k^2R(n^2 - 1)w$

and $\quad \Delta w + k^2 w = - k^2(n^2 - 1)w$

so $\quad \Delta w + k^2 n^2 w = 0$

where $\quad$ w satisfies the radiation condition.

Hence $w \equiv 0$ from the uniqueness of the solution of the original problem and in particular the assumption n is piecewise C^1.

Thus there exists a unique solution $\psi \in H^2(D)$ to the partial differential equation (5.14). Moreover

$$\psi = (I - \tilde{K})^{-1} Rf .$$

From the Fredholm theory $(I - K)^{-1}$ is bounded and R is bounded so that

$$||\psi||_{H^2(D)} \leq C' ||f||_{L^2(D)} .$$

The approach here deals directly with the partial differential equation rather than the equivalent integral formulation. To effect a solution, the interior-exterior problem is treated as a perturbation of a free-space problem. A regularity result for this free-space problem was utilized.

The method of proof in the theorem is more widely applicable than just applying Fredholm theory to the equivalent integral equation formulation. This is because the regularity result for the free space problem may be available from means other than the integral representation.

In particular for vector-valued generalizations of the Helmholtz equation (see §6.6.1) the integral operators involved have strong rather than weak singularities and are not compact as they stand. However, if a regularity result for the free-space problem is available (from pseudo-differential operator theory for example) then the approach of Theorem 5.6 would be applicable.

We note a result for boundary scattering with the solutions of the Helmholtz equation in $H^2(D)$ [i.e. H^2_{loc}] has been proven by Phillips [1973]. Fredholm theory is applied and the use of integral equations is also avoided.

Theorem 5.7 is an extension (the extension being to unbounded domains of the H^2_{loc} regularity of weak solutions for operators on a bounded domain given by Gilbarg and Trudinger [1977] p.183. Theorem 5.7 for solutions in $H^2(D)$ is complimentary to the earlier result also proven using the Fredholm alternative theorem (and the equivalent integral formulation), where the field belonged to the space $C^1(\overline{D})$. That particular regularity result is used in the next chapter on the inverse problem. There the Fréchet differentiability of the refractive index to field map is proven for continuous refractive indices. Similarly, Fréchet differentiability could also be shown using the Sobolev space regularity theory just obtained for piecewise C^1 indices.

5.5 NUMERICAL SOLUTIONS

The methods we propose in the next chapter for solving an inverse problem for the modified Helmholtz equation, require the numerical solution of the direct problem with arbitrary refractive index. This motivates us to review the schemes that are available from the literature for such a numerical solution. Also, the regularity theory derived by the direct problem in the previous section is aimed at finite element solutions.

With a low wave number/frequency it is clearly preferable to utilize the Neumann series approach of §5.3 to solve the modified Helmholtz equation. Johnson and Tracy [1983] do this when using an iterative method to solve the inverse problem.

At high frequencies asymptotic methods from geometric optics may be utilized - these are outlined in Chapter Seven.

However, at intermediate frequencies, some sort of finite element solution of the problem is necessary. We shall outline a few possible approaches of this form. One method could be to solve the volume integral equation formulation of the modified Helmholtz equation using a finite element method. The weak singularity from the Green function in the kernel must be taken into account. However this scheme would be relatively expensive due to the integrals over the region Ω and the full matrix equations that are obtained.

The alternative is to attack the partial differential equation directly. In the interior of the region Ω the solution may be represented by finite elements - that is, as a sum of suitable piecewise polynomial basis functions. However, clearly this is not possible for the whole of $\mathbb{R}^n$. This requires the use of some other method to represent the solution outside Ω, where as n = 1 the Helmholtz equation proper is satisfied.

Firstly separated variable solutions of the Helmholtz equation could be used, with some matching across $\partial\Omega$. The completeness of the separated variable solutions in $L^2(\partial\Omega)$ is established in Colton [1980] pp.130-133. For some numerical computations using this approach see Chen and Mei [1975], who solved a problem for water waves. Alternatively, the solution outside Ω can be represented by a boundary integral equation on $\partial\Omega$. This may be derived from the integral representation for solutions of the free-space Helmholtz equation (see Williams [1980] p.285 for example).

These two methods result in a system of equations with a relatively small full submatrix (from the matching of the separated variable solutions or the boundary integral equation) imbedded in a sparse matrix (resulting from the finite element approximation in Ω). An approach which preserves the sparsity of the system of equations is a matching of the conventional finite element solution inside Ω to a finite element solution in a large but finite outer region enclosing Ω. The radiation condition is then applied at the distant, but finite boundary, of the outer region.

Such a method incorporating a wavelike variation in the shape functions has been utilized by Astley [1983] (see also Astley and Eversman [1983]). Their technique approximates many wavelengths of the solution with a single element. It also includes features of ray optic behaviour with the boundaries of the elements being formed by ray paths and lines of constant phase (or approximations to them).

We note here that Costabel and Stephen [1978] have proven convergence results for the coupling of finite elements and boundary elements for transmission problems in the elastic wave case.

CHAPTER SIX

INVERSE REFRACTIVE INDEX SCATTERING

6.1 INTRODUCTION

In this chapter the inverse problem of determining a spatially varying refractive index in the Helmholtz equation is examined. This problem has been investigated by various authors - see Bates [1984] for example.

The direct scattering problem

$$\psi = \psi^i + \psi^s \quad , \quad \underset{\sim}{x} \in \mathbb{R}^n \, , \, n = 2, 3$$

$$\Delta\psi + k^2 n^2 \psi = 0 \quad , \quad \underset{\sim}{x} \in \mathbb{R}^n$$

and

$$\frac{\partial\psi^s}{\partial|\underset{\sim}{x}|} - ik\psi^s \sim o(|\underset{\sim}{x}|)^{\frac{1-n}{2}} \quad , \text{ as } \underset{\sim}{x} \to \infty \; ,$$

was considered in the previous chapter.

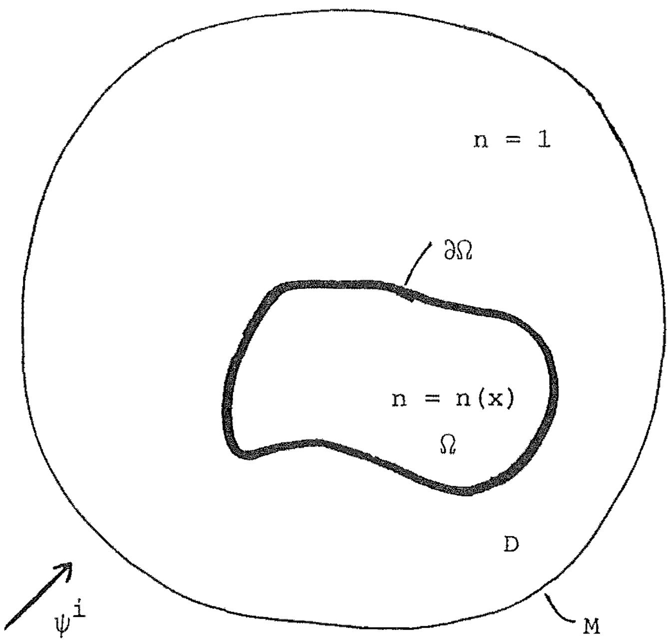

Figure 6.1

The refractive index is unity outside Ω, a region of compact support. The boundary $\partial\Omega$ is assumed to be known and the problem at a fixed wave number, k, will be considered.

A set of linearly independent fields

$$\{\psi_p^i(\underline{x})\} \quad , \quad p \in \{1, ..., N\}$$

is used to probe the scatterer. Measurements of the resulting fields $\{\psi_p(\underline{x})\}$ are made on a surface M exterior to Ω. The region inside M shall be denoted by D. We consider later the case where the farfield pattern is known instead.

The extension of our methods to the case where the measurements are performed at varying frequencies can easily be made, but will not be outlined here.

The alternative problem of determining the shape and location of an unknown scattering boundary, $\partial\Omega$, was examined in Chapter Four.

6.1.1 *Uniqueness*

It has been known for sometime that a radially (or spherically) symmetric refractive index may be uniquely reconstructed from scattering data at a single frequency - see Chadan and Sabatier [1977].

We shall see after that the linearized version of the inverse problem (i.e. within the so called Born approximation) is uniquely solvable for a two or three dimensional refractive index.

There is actually a nonlinear transformation between the steady-state diffusion equation

$$\nabla \cdot (f \nabla \phi) = 0$$

and a Helmholtz type equation. Setting

$$\psi = f^{\frac{1}{2}}\phi$$

and

$$q = \frac{\Delta(f^{\frac{1}{2}})}{f^{\frac{1}{2}}}$$

then

$$\Delta\psi + q\psi = 0 \ .$$

Sylvester and Uhlmann [1986] have used the transformation in proving a uniqueness result for the inverse problem of determining functions q close enough to zero in the above equation. The equation is defined on a bounded region and has Dirichlet data. They extend their uniqueness result for the inverse problem of the steady-state diffusion equation with a nearly constant coefficient.

More recently Ramm [1987c, 1988] has shown there is a unique solution to the full nonlinear inverse problem - at a single frequency and for three-dimensional $n \in L^{\infty}$. The proof is based upon the completeness of solutions to the partial differential equation. We examine this result in more detail later in §6.4.

6.1.2 *Preview*

In the next section we formulate the inverse problem as a nonlinear operator equation and investigate the use of the Newton-Kantorovich method to solve this. A closely related scheme due to Johnson and Tracy is then examined. They produce some numerical reconstructions of a two-dimensional object.

In §6.3 we prove some Fréchet differentiability results for the nonlinear operator. A Lipschitz continuity result is then also obtained. Finally the regularization of the problem is considered.

The measurement of the farfield pattern is examined in §6.4. The Fréche derivative is derived and then formally justified. The inversion of the Bor approximation with farfield measurements is then reviewed. The use of th steepest descent method is outlined in §6.5, for minimizing an appropriat functional arising from farfield measurements.

In §6.6 the solution of the corresponding inverse problem for the Riccat wave equation, a nonlinear form of the Helmholtz equation, is considered. Th use of the Rytov approximation for this problem is then investigated.

Finally, in the last section several inverse problems closely related to tha for the Helmholtz equation are examined. Vector generalizations of th Helmholtz equation are considered, then a time domain inverse problem for th wave equation.

6.2 NONLINEAR OPERATOR APPROACH

6.2.1 *Newton–Kantorovich Method*

We now outline the application of the Newton-Kantorovich method for solving this inverse problem. Setting $\nu \equiv n^2$ the nonlinear operator equation to be solved is

$$U(\nu) = \psi_p(\nu;\underline{x}) - \Psi_p(\underline{x}) = 0\,, \qquad \underline{x} \in M,\ p \in \{1,\dots,N\}\ . \tag{6.1}$$

Here $\psi_p(\nu;\underline{x})$ is the field resulting from the incident field $\psi_p^i(\underline{x})$, and the refractive index squared, ν. $\Psi_p(\underline{x})$ is the field that is measured on M.

Differentiating the direct problem formulation with respect to ν gives

$$\Delta\psi'(\nu)s \ + \ k^2\nu\psi'(\nu)s = - k^2\psi(\nu)s$$

and

$$\frac{\partial}{\partial|\underline{x}|}[\psi'(\nu)s] - ik\psi'(\nu)s \sim o(|\underline{x}|)^{\frac{1-n}{2}}, \ \text{as } |\underline{x}| \to \infty \ .$$

That is, the Fréchet differential $\psi'(\nu)s$ satisfies the Helmholtz equation with the addition of a source term, and also the radiation condition.

Thus using the integral representation for the solution (5.3)

$$\psi'(\nu)s = k^2\int_\Omega G(\nu;\underline{x},\underline{x}')\ \psi(\nu;\underline{x}')\ s(\underline{x}')\ dV' \ , \ \underline{x} \in \mathbb{R}^n . \tag{6.2}$$

Here the Green function $G(\nu)$ satisfies

$$G(\nu;\underline{x},\underline{x}') + k^2\nu(\underline{x})\ G(\nu;\underline{x},\underline{x}') = \delta(\underline{x}-\underline{x}') \ , \ \underline{x} \in \mathbb{R}^n$$

and the radiation condition.

The update $s^{(k)}(\underline{x})$ in the Newton-Kantorovich method is then from (6.1) and (6.2) the solution of the integral equation

$$k^2\int_\Omega G(\nu^{(k)};\underline{x},\underline{x}')\ \psi(\nu^{(k)};\underline{x}')\ s^{(k)}(\underline{x}')\ dV' = \Psi_p(\underline{x}) - \psi_p(\nu^{(k)};\underline{x}) \ ,$$

$$\underline{x} \in M, \ p \in \{1,...,N\} \ . \tag{6.3}$$

We prove a Fréchet differentiability result to formalize this in the next section.

Similar schemes have been used to reconstruct one-dimensional refractive indices in inverse scattering problems at one frequency by Roger [1978] and Tsien and Chen [1978] and with many frequencies by Coen *et al.* [1981].

We note that if an initial approximation $\nu^{(0)} = 1$ is chosen, then the integral equation (6.3) becomes

$$k^2 \int_{\Omega} G_0(\underset{\sim}{x},\underset{\sim}{x}')\, \psi^i(\underset{\sim}{x}')\, s^{(1)}(\underset{\sim}{x}')\, dV' = \Psi_p(\underset{\sim}{x}) - \psi^i(\underset{\sim}{x}) ,$$

$$\underset{\sim}{x} \in M ,\ p \in \{1,\ldots,N\} . \qquad (6.4)$$

This equation is similar in form to that from the Born approximation (5.13). Except here the equation (6.4) gives an approximate solution, $\nu(\underset{\sim}{x}) = 1 + s^{(1)}(\underset{\sim}{x})$, to the inverse problem.

6.2.2 *Alternative Schemes*

The original iterative method for this inverse problem is due to Jost and Kohn [1952] - see also Moses [1956] and Prosser [1969, 1976, 1980]. Their scheme inverts the Born series resulting from the Schrodinger equation (or alternatively the Helmholtz equation - THEOREM 5.4). It is then only applicable to determining weak potentials or refractive indices close enough to unity. Scattering data is required for a variable frequency by these authors, however Devaney and Wolf [1982] consider the single frequency case. The only numerical results available from this method are in one dimension.

The only fully two-dimensional reconstructions for this problem using an iterative method (to date), have been performed by Johnson and Tracy [1983], Tracy and Johnson [1983] and Johnson *et al.* [1984]. They use the following procedure.

Set $\gamma = n^2 - 1$. Then these two equations of theirs describe the inverse problem :

$$\Psi_p(\underline{x}) - \psi_p^i(\underline{x}) = k^2 \int_\Omega G_0(\underline{x},\underline{x}') \, \psi_p(\underline{x}') \, \gamma(\underline{x}') \, dV' \ , \ \underline{x} \in M, \ p \in \{1,...,N\}$$

$$\psi_p(\underline{x}) - \psi_p^i(\underline{x}) = k^2 \int_\Omega G_0(\underline{x},\underline{x}') \, \psi_p(\underline{x}') \, \gamma(\underline{x}') \, dV' \ , \ \underline{x} \in \Omega, \ p \in \{1,...,N\} \ . \tag{6.5}$$

Like us, they utilize a set of different incident fields to obtain the measurements $\Psi_p(\underline{x})$, $p \in \{1,...N\}$. The two equations above arise from the integral equation (5.4).

The first relates the measurements to the field and refractive index. The second is the integral equation defining the direct problem solution for the field.

They regard them as a system of nonlinear integral equations to be solved for the N+1 functions γ and $\{\psi_p\}$, $p \in \{1,...,N\}$. The unknown functions are discretized giving a system of nonlinear algebraic equations. These are then solved using a variety of iterative methods including steepest descent.

Their approach is different to ours in that we first formulate the problem as a nonlinear operator equation for ν and γ alone. Then the direct problem solutions ψ_p are computed from γ at each iteration. However, the two approaches are related in the following manner.

In each of their papers one iterative scheme used to solve the system (6.5) is the alternating variable method. For this method given an approximation to the $\{\psi_p\}$, the first equation is solved for γ. Then given this approximation to γ the second equation is solved for each of the ψ_p. The process is then repeated in an iterative manner.

This solving of an integral equation of the first kind for the refractive index, then solving direct problems for the fields ψ_p, at each iteration, is similar to the iterative schemes we propose. Let us investigate this relationship more closely.

Their iterative scheme becomes the following.

(1) Given an approximation $\gamma^{(k)}$, solve for the $\psi_p(\gamma^{(k)})$:

$$\psi(\gamma^{(k)}) - \psi_p^i = k^2 \int_\Omega G_0 \psi(\gamma^{(k)}) \, \gamma^{(k)} \, dV' \quad .$$

(2) Then solve for new approximation $\gamma^{(k+1)}$:

$$\Psi_p - \psi_p^i = k^2 \int_\Omega G_0 \, \psi_p(\gamma^{(k)}) \, \gamma^{(k+1)} \, dV' \ , \ \underset{\sim}{x} \in M \, .$$

Subtracting these two equations gives

$$\Psi_p - \psi_p(\gamma^{(k)}) = k^2 \int_\Omega G_0 \psi(\gamma^{(k)})[\gamma^{(k+1)} - \gamma^{(k)}] \, dV' \ , \ \underset{\sim}{x} \in M \, .$$

or

$$\Psi_p - \psi_p(\nu^{(k)}) = k^2 \int_\Omega G_0 \, \psi(\nu^{(k)})[\nu^{(k+1)} - \nu^{(k)}] \, dV', \underset{\sim}{x} \in M. \tag{6.6}$$

This last equation is to be solved for the new approximation at each iteration $\nu^{(k+1)}$. It is a similar integral equation to that which we solve at each iteration in the Newton-Kantorovich method. However instead of updating the Green function in the kernel to $G(\nu^{(k)})$ at each iteration, the Green function is left fixed at $G_0 = G(\nu)$ when $\nu \equiv 1$. The modified form of the Newton-Kantorovich with initial approximation $\nu^{(0)} = 1$ would have the Green function fixed at G_0, but the field in the kernel would also be left fixed at $\psi^i = \psi(\nu)$ when $\nu = 1$. The field inside the Johnson and Tracy integral equation is updated at each iteration to $\psi(\nu^{(k)})$. Thus the alternating variable iterative scheme of Johnson and Tracy lies somewhere between the modified form of the

Newton-Kantorovich method and the Newton-Kantorovich method proper in that the kernel is only partially updated at each iteration. All these iterative schemes have the Born approximation as the first iteration.

They reconstruct refractive indices close enough to unity such that Neumann series may be used to solve the direct problems. The last paper, Johnson *et al.* [1984] investigates fast methods of implementing the iterative scheme just outlined. The use of back projection methods is examined for solving the first kind integral equations for the refractive index and the Fast Fourier Transform (F.F.T.) is utilized in solving the direct problems.

The object reconstructed is a two-dimensional Gaussian distribution with the refractive index squared taking on values between 1.1 and 1. That is, there is a 10% maximum variation on a unity refractive index.

The maximum error in the reconstructions is $0.0001 = 10^{-4}$. This is much superior to what could be expected from using the Born approximation (which is just one iteration of the scheme). As the Born approximation linearizes the inverse problem, a second order error in the vicinity of $\gamma^2 = 0.01$ would be expected. Even though the object reconstructed is radially symmetric, this is not assumed in the discretization of the problem, and so the reconstruction is a two-dimensional one.

The refractive index reconstructed is fairly close to unity and so we could not expect their algorithm to perform as well for an arbitrary refractive index. Indeed, the Born series method of solving the direct problems only works for refractive indices close enough to unity. Moreover, as a modified type of Newton-Kantorovich method is being used, the scheme may not converge in reconstructing refractive indices that vary far from unity. However, we note here that if the Newton-Kantorovich method proper is used, along with the improvements suggested in §1.4.3, then it would be possible to reconstruct arbitrary refractive indices.

There have been several other iterative solutions of the inverse problem.

Colton and Monk [1988] extend their method for inverse boundary scattering based upon the theory of Herglotz wave functions (reviewed in §4.2.3) to this problem. This approach relies upon determining the normal to the hyperlane of farfield patterns rather than projecting the measured data onto the class of farfield patterns - which we suggest in §6.4.

They reconstructed some one-dimensional refractive indices using a Newton-like method to minimize their functional. However we note their scheme is not applicable at an arbitrary frequency as it stands and requires measurements of both the phase and amplitude. It has not been numerically tested in higher dimensions as yet.

Tan *et al.* [1988] (see also Tan [1988]) obtain a nonlinear system of equations from basis function expansions for both the refractive index and field, with the partial differential equation and scattering data being satisfied. This system is solved using a Newton method, and radially symmetric and simple two-dimensional piecewise constant distributions are reconstructed. The approach is based upon an inverse scattering method of Bates [1984]. Their operator formulation differs from ours, with the Fréchet derivative being difficult to determine explicitly, so that it is computed by finite differences.

We prefer to consider the operator equation (6.1) as it essentially models the physical situation - where the measurements arise as a response to probing by an incident field. The direct problem solution may then be fitted (iteratively) to these measurements using the Newton-Kantorovich method.

It will be shown that one iteration of the Newton-Kantorovich method applied to (6.1) is equivalent to the use of the Born approximation. Thus our approach extends this often used approximate method. We have also shown that a scheme used by Johnson and Tracy to produce two-dimensional reconstructions is equivalent to a modified form of Newton's method.

We note that the Newton-Kantorovich method applied to our operator formulation (combined with a finite element solution of the direct problem), is becoming popular for the solution of the corresponding inverse problem for another elliptic p.d.e., the steady-state diffusion equation - see Connolly and Wall [1988] (which forms the Appendix).

Finally in the next subsection we outline how our scheme may be applied when the phase of the field cannot be measured.

6.2.3 *Phase Problems*

In some practical problems only the amplitude $|\psi|$ of the complex field can be measured, and the phase is unknown. The reconstruction of this phase is known as the phase problem.

With amplitude measurements, $|\Psi|$, the inverse problem may be formulated as a nonlinear operator equation

$$\begin{aligned} W(\nu) &= |\psi(\nu)|^2 - |\Psi|^2 \\ &= \psi(\nu)\,\overline{\psi(\nu)} - |\Psi|^2 = 0 \ , \quad \underset{\sim}{x} \in M \ . \end{aligned} \tag{6.7}$$

Fréchet differentiation with respect to ν gives

$$W'(\nu)s = \psi(\nu)\,\overline{\psi'(\nu)s} + \overline{\psi(\nu)}\,\psi'(\nu)s \tag{6.8}$$

and the Newton-Kantorovich method may be applied to the operator equation (6.7) with $\psi'(\nu)s$ computed as in §6.1. However, the question of uniqueness of solutions becomes even more difficult than when the phase is known.

A similar approach has been used by Coen *et al.* [1981] in solving for one-dimensional refractive indices in an inverse scattering problem. Rather than the operator equation above, they solve

$$\ln|\psi(\nu)| - \ln|\Psi| = 0$$

using an iterative method.

Wall *et al.* [1985] and Murch *et al.* [1988] also consider the analogous problem for inverse boundary scattering when the phase of the measured field is unknown. An operator equation of the form of (6.7) is solved.

In some linearized inverse problems - such as when the Born approximation is utilized (see §6.3) - there is a Fourier transform relationship between the field and the refractive index. Then the nonlinear equation to be solved is

$$|F\nu| = |\Psi| \ , \tag{6.9}$$

where $F\nu$ is the n-dimensional Fourier transform of ν.

This is known as the Fourier phase problem (Bates and McDonnell [1986], Chapter Four) and is generally solved subject to constraints such as positivity of the solution. These are necessary to obtain a unique solution or *image–form.* For an examination of such phase problems in inverse problems see Bates and Tan [1985] and Tan [1988].

The Fourier phase problem is usually solved by iterative methods which obtain solutions as a sequence of Fourier transforms. These can be implemented comparatively cheaply using F.F.T's. The original algorithm is due to Fienup [1978].

In this special case of the phase problem, the Newton-Kantorovich method (which requires the solution of a system of equations at each iteration as well as the imposition of constraints) is unlikely to be competitive, as the problems solved are usually of a large scale requiring excessive storage. This is even though the iterative techniques used to date for the Fourier phase problem are based on projected constraint steepest descent and many thousands of iterations are necessary with such schemes.

6.3 THEORETICAL CONSIDERATIONS

In this section the Fréchet differentiability of the refractive index to field map is proven using regularity theory from Chapter Five.

Firstly, such a differentiability result is shown for continuous refractive indices and a continuously differentiable field. Then Fréchet differentiability within the regularity theory for the Born series is proven and this is used to formalize the Born approximation.

A result for the Lipshitz continuity of the map is then proven - within the Born series theory. The compactness of the Fréchet derivative with point measurements is also established. This ensures that the solution of the inverse problem is unstable in the presence of measurement noise. So finally in this section the regularization of the problem is examined.

6.3.1 *Fréchet Differentiability*

In this subsection we prove Fréchet differentiability for the operator equation (6.1) - within the regularity theory of the last chapter which made use of the Fredholm alternative theorem.

Consider $\nu = n^2$ belonging to the open set $X_0 = \{\nu : \nu \in C^0(\overline{\Omega}), \nu > 0\}$. From THEOREM 5.1 if $\nu \in X_0$ then there exists a unique solution $\psi \in C^1(\overline{D})$ of the integral equation (5.4). All sources are required to be external to the compact domain D. We then have the following.

THEOREM 6.1

The map $\nu \to \psi(\nu)$ from $X_0 \to C^1(\overline{D})$ is Fréchet differentiable with

$$\psi'(\nu)s = k^2 \int_{\Omega} G(\nu;\underset{\sim}{x},\underset{\sim}{x}') \, \psi(\nu;\underset{\sim}{x}') \, s(\underset{\sim}{x}') \, dV' \quad . \tag{6.18}$$

<u>Proof</u> The implicit function theorem (see §1.5.3) shall be used to obtain the desired result. $\xi(\nu,\psi)$ is obtained from the integral equation formulation of the direct problem, i.e. set

$$\xi(\nu,\psi) = \psi - \psi^{i} - k^2 \int_{\Omega} G_0(\nu-1) \, \psi \, dV'$$

$$= \psi - \psi^{i} - \overline{K}(\nu-1) \, \psi \quad .$$

Then $\xi : X_0 \otimes C^1(\overline{D}) \to C^1(\overline{D})$ (see LEMMA 5.2).

We now check the conditions of the implicit function theorem.

1. $$\delta\xi = \xi(\nu+\delta\nu, \psi+\delta\psi) - \xi(\nu,\psi)$$

$$= \delta\psi - \overline{K}(\delta\nu\psi + (\nu-1)\,\delta\psi + \delta\nu\delta\psi)$$

giving

$$||\delta\xi||_{C^1(\overline{D})} \leq ||\delta\psi||_{C^1(\overline{D})} + ||\overline{K}|| \;\; ||\delta\nu\psi + (\nu-1)\delta\psi + \delta\nu\delta\psi||_{C^0(\overline{\Omega})}$$

as $\overline{K} : C^0(\overline{\Omega}) \to C^1(\overline{D})$.

The operator norm $||\overline{K}||$ is as defined in Chapter Five.

Hence

$$\begin{aligned}
||\delta\xi||_{C^1(\overline{D})} &\le ||\delta\psi||_{C^1(\overline{D})} + ||\overline{K}||(||\delta\nu||_{C^0(\overline{\Omega})}||\psi||_{C^0(\overline{\Omega})} \\
&\qquad + ||\nu\text{-}1||_{C^0(\overline{\Omega})}||\delta\psi||_{C^0(\overline{\Omega})} + ||\delta\nu||_{C^0(\overline{\Omega})}||\delta\psi||_{C^0(\overline{\Omega})}) \\
&\le ||\delta\psi||_{C^1(\overline{D})} + ||\overline{K}||(||\delta\nu||_{C^0(\overline{\Omega})}\ ||\psi||_{C^1(\overline{D})} \\
&\qquad + ||\nu\text{-}1||_{C^0(\overline{\Omega})}\ ||\delta\psi||_{C^1(\overline{D})} + ||\delta\nu||_{C^0(\overline{\Omega})}\ ||\delta\psi||_{C^1(\overline{D})})
\end{aligned}$$

as $||\psi||_{C^0(\overline{\Omega})} \le ||\psi||_{C^1(\overline{D})}$.

Now $||\delta\xi||_{C^1(\overline{D})} \to 0$ as $||\delta\nu||_{C^0(\overline{\Omega})}, ||\delta\psi||_{C^1(\overline{D})} \to 0$
so ξ is continuous in ν and ψ .

2. The partial Fréchet derivative of ξ w.r.t. ν is

$$\xi_\nu(\nu,\psi)s = -\overline{K}\psi s \ ,$$

where $s \in C^0(\overline{\Omega})$.

So

$$\begin{aligned}
&||\xi_\nu(\nu+\delta\nu,\ \psi+\delta\psi)s - \xi_\nu(\nu,\psi)s||_{C^1(\overline{D})} \\
&\qquad = ||\overline{K}\delta\psi s||_{C^1(\overline{D})} \\
&\qquad \le ||\overline{K}||\ \ ||\delta\psi s||_{C^0(\overline{\Omega})} \\
&\qquad \le ||\overline{K}||\ \ ||\delta\psi||_{C^1(\overline{D})}\ ||s||_{C^0(\overline{\Omega})} \ .
\end{aligned}$$

Thus $\xi_{\nu}(\nu,\psi)$ is continuous in ν and ψ. The partial Fréchet derivative of ξ w.r.t. ψ is

$$\xi_{\psi}(\nu,\psi)t = t - \overline{K}(\nu\text{-}1)t$$

where $t \in C^1(\overline{\Omega})$, and so $\xi_{\psi}(\nu,\psi)$ may be shown to be continuous in ν and ψ in a similar manner to ξ_{ν}.

3. $[\xi_{\psi}(\nu,\psi)]^{-1}$ is bounded from THEOREM 5.2.

The conditions of the implicit function theorem (THEOREM 1.1) are then satisfied and

$$\begin{aligned}\psi'(\nu)s &= -[\xi_{\psi}(\nu,\psi)]^{-1}\,\xi_{\nu}(\nu,\psi)s \\ &= [I - \overline{K}(\nu\text{-}1)]^{-1}\,\overline{K}\,\psi s\ ,\end{aligned} \tag{6.19}$$

so we have at this point the integral equation satisfied by the Fréchet derivative.

To get the explicit expression (6.10) for the Fréchet derivative, we first show that

$$u(\underset{\sim}{x}) = \int_{\Omega} G(\nu;\underset{\sim}{x},\underset{\sim}{x}')\,\rho(\underset{\sim}{x}')dV'$$

is equivalent to

$$u = [I - K(\nu\text{-}1)]^{-1}\,\overline{K}\rho\ .$$

That is $\quad u = k^2\int_{\Omega} G(\nu)\rho\, dV' \quad$ is the solution of

$$u - \overline{K}(\nu\text{-}1)u = \overline{K}\rho$$

or $$u(\underset{\sim}{x}) = k^2\int_\Omega G_0(\underset{\sim}{x},\underset{\sim}{x}')[\nu(\underset{\sim}{x}') - 1]\, u(\underset{\sim}{x}')dV' + k^2\int_\Omega G_0(\underset{\sim}{x},\underset{\sim}{x}')\rho(\underset{\sim}{x}')dV'. \qquad (6.20)$$

From (5.5) the Green function $G(\nu)$ satisfies the following integral equation

$$G(\nu;\underset{\sim}{x},\underset{\sim}{x}') = G_0(\underset{\sim}{x},\underset{\sim}{x}') + k^2\int_\Omega G_0(\underset{\sim}{x},\underset{\sim}{x}'')\; G(\nu;\underset{\sim}{x}'',\underset{\sim}{x}')[\nu(\underset{\sim}{x}'')-1]dV'' \;.$$

So

$$\begin{aligned} u(\underset{\sim}{x}) &= k^2\int_\Omega G(\nu;\underset{\sim}{x},\underset{\sim}{x}')\rho(\underset{\sim}{x}')dV' \\ &= k^2\int_\Omega G_0(\underset{\sim}{x},\underset{\sim}{x}')\rho(\underset{\sim}{x}')dV' + k^2\int_\Omega \left[k^2\int_\Omega G_0(\underset{\sim}{x},\underset{\sim}{x}'')G(\nu;\underset{\sim}{x}'',\underset{\sim}{x}')[\nu(\underset{\sim}{x}'')-1]dV''\right]\rho(\underset{\sim}{x}')dV' \\ &= k^2\int_\Omega G_0(\underset{\sim}{x},\underset{\sim}{x}')\rho(\underset{\sim}{x}')dV' + k^2\int_\Omega G_0(\underset{\sim}{x},\underset{\sim}{x}'')\left[k^2G(\nu;\underset{\sim}{x}'',\underset{\sim}{x}')\rho(\underset{\sim}{x}')dV'\right][\nu(x'')-1]dV'' \\ &= k^2\int_\Omega G_0(\underset{\sim}{x},\underset{\sim}{x}')\rho(\underset{\sim}{x}')dV' + k^2\int_\Omega G_0(\underset{\sim}{x},\underset{\sim}{x}'')u(\underset{\sim}{x}'')[\nu(\underset{\sim}{x}'')-1]dV'' \end{aligned}$$

as required for (6.20). The interchange in the integral is justified by Fubini's theorem - see Miklin [1970] p.86, where such an integral with a weak singularity is considered.

Setting $\rho = \psi s$ in (6.19) gives

$$\begin{aligned} \psi'(\nu)s &= [I - \overline{K}(\nu\text{-}1)]^{-1}\, \overline{K}\psi s \\ &= \int_\Omega G(\nu;\underset{\sim}{x},\underset{\sim}{x}')\psi(\underset{\sim}{x}')s(\underset{\sim}{x}')dV' \;. \qquad \square \end{aligned}$$

So the operator equation (6.1) is indeed Fréchet differentiable, moreover the expression for the Fréchet derivative we derived in §6.1 in a fairly intuitive manner is correct. That derivation utilized the partial differential equation rather than the integral equation form.

6.3.2 *Born Series Result*

Now we shall show Fréchet differentiability within the regularity theory obtained when the Born series converges - see §5.3. This has the advantage, over the result just derived, that continuity of the refractive index is not required. However, there is of course a restriction on the size of the L^2 norm of ν-1 = n^2-1.

In addition, we formalize the Born approximation (6.4) as the Fréchet derivative (that is, the formal linearization) of the refractive index to field map, about a unity refractive index. This view differs from that of most authors who consider the Born approximation as an approximate solution of the direct problem, and then use this to obtain an approximate solution of the inverse problem.

Consider ν belonging to the open set X_2 defined as follows :
$X_2 = \{\nu : \nu \in L^2(\Omega),\ ||\nu-1||_{2,\Omega} < 1/||K||\}$. From THEOREM 5.6 it follows $||K|| = ak^2$ for Ω a sphere of radius a.

LEMMA 6.1 If $\nu \in X_2$ then there exists a unique solution $\psi \in C^0(\overline{D})$ of (5.4). Moreover

$$||\psi||_{C^0(\overline{D})} \leq \eta||\psi^i||_{C^0(\overline{D})} \quad .$$

<u>Proof</u> Since $\nu \in X_2$ $\quad ||K||\ ||\nu-1||_2 < 1$.

But $\quad ||K(\nu-1)|| \leq ||K||\ ||\nu-1||_2$ [from LEMMA 5.2 (ii)]

and so $\quad ||K(\nu-1)|| < 1$.

Then from THEOREM 5.4 and COROLLARY 5.1 there exists a unique solution $\psi \in C^0(\overline{D})$.

Now
$$\psi = \psi^{i} + \int_{\Omega} G_0(\nu-1)\psi \, dV'$$

or

$$\psi = \psi^{i} + K'(\nu-1)\psi$$

where $K' : L^2(\Omega) \to C^0(\overline{D})$ [c.f. $K : L^2(\Omega) \to C^0(\overline{\Omega})$] .

So

$$\|\psi\|_{C^0(\overline{D})} \leq \|\psi^{i}\|_{C^0(\overline{D})} + \|K'\| \, \|(\nu-1)\psi\|_{L^2(\Omega)}$$

$$\leq \|\psi^{i}\|_{C^0(\overline{D})} + \|K'\| \, \|\nu-1\|_2 \, \|\psi\|_{C^0(\overline{\Omega})} \, . \tag{6.21}$$

But from THEOREM 5.4

$$\|\psi\|_{C^0(\overline{\Omega})} \leq \frac{\|\psi^{i}\|_{C^0(\overline{\Omega})}}{1 - \|K\| \, \|\nu-1\|_2}$$

$$\leq \frac{\|\psi^{i}\|_{C^0(\overline{D})}}{1 - \|K\| \, \|\nu-1\|_2}$$

as $\|\psi^{i}\|_{C^0(\overline{\Omega})} \leq \|\psi^{i}\|_{C^0(\overline{D})}$.

So from (6.21)

$$\|\psi\|_{C^0(\overline{D})} \leq \|\psi^{i}\|_{C^0(\overline{D})} + \frac{\|K'\| \, \|(\nu-1)\|_2 \, \|\psi^{i}\|_{C^0(\overline{D})}}{1 - \|K\| \, \|\nu-1\|_2}$$

$$= \left[1 + \frac{\|K'\| \, \|\nu-1\|_2}{1 - \|K\| \, \|\nu-1\|_2}\right] \|\psi^{i}\|_{C^0(\overline{D})}$$

as required. □

We now have the necessary regularity result to prove the following :

THEOREM 6.2

The map $\nu \to \psi(\nu)$ from $X_2 \to C^0(\overline{D})$ is Fréchet differentiable.

Proof Again the implicit function theorem (see §1.5.3) will be used to produce the desired result.

As before we set

$$\begin{aligned}\xi(\nu,\psi) &= \psi - \psi^{i} - k^2 \int_{\Omega} G_0(\nu-1)\psi dV' \\ &= \psi - \psi^{i} - K'(\nu-1)\psi, \text{ where } K' : L^2(\Omega) \to C^0(\overline{D}) .\end{aligned}$$

Then $\xi : X_2 \otimes C^0(\overline{D}) \to C^0(\overline{D})$. We now check the conditions of the theorem.

1. $$\begin{aligned}\delta\xi &= \xi(\nu+\delta\nu, \psi+\delta\psi) - \xi(\nu,\psi) \\ &= \delta\psi - K'(\delta\nu\psi + (\nu-1)\delta\psi + \delta\nu\delta\psi)\end{aligned}$$

So

$$\|\delta\xi\|_{C^0(\overline{D})} \leq \|\delta\psi\|_{C^0(\overline{D})} + \|K'\| \; \|\delta\nu\psi + (\nu-1)\delta\psi + \delta\nu\delta\psi\|_{L^2(\Omega)}$$

$$\text{as } K' : L^2(\Omega) \to C^0(\overline{D}) .$$

Hence

$$\begin{aligned}\|\delta\xi\|_{C^0(\overline{D})} &\leq \|\delta\psi\|_{C^0(\overline{D})} + \|K'\|(\|\delta\nu\|_2\|\psi\|_{C^0(\overline{\Omega})} + \|\nu-1\|_2\|\delta\psi\|_{C^0(\overline{\Omega})} \\ &\qquad + \|\delta\nu\|_2\|\psi\|_{C^0(\overline{\Omega})}) \\ &\leq \|\delta\psi\|_{C^0(\overline{D})} + \|K'\|(\|\delta\nu\|_2\|\psi\|_{C^0(\overline{D})} + \|\nu-1\|_2\|\delta\psi\|_{C^0(\overline{D})} \\ &\qquad + \|\delta\nu\|_2\|\delta\psi\|_{C^0(\overline{D})})\end{aligned}$$

because $\|\psi\|_{C^0(\overline{\Omega})} \leq \|\psi\|_{C^0(\overline{D})}$.

Now $||\delta\xi||_{C^0(\overline{D})} \to 0$ as $||\delta\nu||_{L^2(\Omega)}$, $||\delta\psi||_{C^0(\overline{D})} \to 0$
so ξ is continuous in ν and ψ.

2. $\xi_\nu(\nu,\psi) = - K'\psi s,$ where $s \in L^2(\Omega)$.

So
$$||\xi_\nu(\nu+\delta\nu,\ \psi+\delta\psi)s - \xi_\nu(\nu,\psi)s||_{C^0(\overline{D})}$$
$$= ||K'\,\delta\psi s||_{C^0(\overline{D})}$$
$$\leq ||K'||\ ||\delta\psi s||_{L^2(\Omega)}$$
$$\leq ||K'||\ ||\delta\psi||_{C^0(\overline{D})}\ ||s||_{L^2(\Omega)}\ .$$

Thus ξ_ν is continuous in ν and ψ.

Also
$$\xi_\psi(\nu,\psi)t = t - K'(\nu\text{-}1)t, \quad \text{where } t \in C^0(\overline{\Omega})\ .$$

$\xi_\psi(\nu,\psi)$ may then be shown to be continuous in ν and ψ in a similar manner to ξ_ν.

3. $[\xi_\psi(,\psi)]^{-1}$ is bounded from LEMMA 6.1.

The conditions of the implicit function theorem (THEOREM 1.1) are then satisfied.

Moreover
$$\psi'(\nu)s = - [\xi_\psi(\nu,\psi)]^{-1}\ \xi_\nu(\nu,\psi)s$$
$$= \quad [I - K'(\nu\text{-}1)]^{-1}\ K'\psi s\ . \qquad \square$$

The expression for the Fréchet derivative just derived takes the form of a series like the solution of the direct problem.

However, the Fréchet derivative at a refractive index of unity simplifies somewhat.

COROLLARY 6.1 When $\nu = 1$

$$\begin{aligned} \psi'(\nu)s &= K'\psi^{i}s \\ &= k^2 \int_{\Omega} G_0 \psi^{i} s \, dV' \ , \end{aligned}$$

with $\psi'(1) : L^2(\Omega) \to C^0(\overline{D})$. □

This Corollary shows that the Born approximation (6.4) gives the formal linearization of $\psi(\nu)$ about a refractive index of unity. Most other authors consider the Born approximation to be an approximate solution of the direct problem - obtained as the leading term of the Born (or Neumann) series. This then provides a linear integral equation to solve for an approximate solution to the inverse problem. We have shown that their particular linearization is in fact the Fréchet derivative (i.e. a uniform linear approximation) to our operator equation, about a unity index.

The two Fréchet differentiability results proven in this section so far are complementary. The result in the first subsection gives differentiability for continuous refractive indices of arbitrary distance from unity. The result of this subsection only requires the refractive index to be square integrable (discontinuities are allowed) however it must be sufficiently close to unity.

6.3.3 *Lipschitz Continuity*

Weston [1979] has proved a Lipschitz continuity result using the regularity theory for continuous refractive indices. This was for the following compact subset of $C^0(\overline{\Omega})$

$$S' = \{\nu : \nu \in C^0(\overline{\Omega}) \, , \, \|\nu\|_{\infty} \leq \alpha \, , \, \nu \text{ equicontinuous}\} \ .$$

We shall prove a Lipschitz continuity result within the Born series regularity theory. This will only require ν to belong to a bounded subset of $L_2(\Omega)$ (rather than a compact one)

$$X_1 = \{\nu : \nu \in L_2(\Omega) \, , \, \|\nu-1\|_{2,\Omega} \leq M < 1/\|K\|\} \, .$$

THEOREM 6.3

The map $\nu \to \psi(\nu)$ from $X_1 \to C^0(\overline{D})$ is Lipschitz continuous.

Proof To prove the result we must show (see §1.5.4)

$$\|\psi(\nu+\delta\nu) - \psi(\nu)\|_{C^0(\overline{D})} \leq N_0\|\delta\nu\|_{2,\Omega}$$

where N_0 is independent of ν. That is, N_0 depends only upon M, the incident field ψ^i and the regions Ω and D.

Now

$$\psi(\nu) = \psi^i + K^2\int_\Omega G_0(\nu-1)\psi(\nu)\, dV'$$

or

$$\psi(\nu) = \psi^i + K'(\nu-1)\psi(\nu) \, .$$

Also

$$\psi(\nu+\delta\nu) = \psi^i + K'(\nu+\delta\nu-1)\psi(\nu+\delta\nu) \, .$$

Subtracting gives

$$\psi(\nu+\delta\nu) - \psi(\nu) = K'(\nu+\delta\nu-1)[\psi(\nu+\delta\nu)-\psi(\nu)] + K'\delta\nu\psi(\nu)$$

or

$$[I - K'(\nu+\delta\nu-1)]\,[\psi(\nu+\delta\nu)-\psi(\nu)] = K'\delta\nu\psi(\nu) \, .$$

Now from LEMMA 6.1 $[I + K(\nu+\delta\nu-1)]^{-1}$ is bounded, giving

$$\begin{aligned} \|\psi(\nu+\delta\nu)-\psi(\nu)\|_{C^0(\overline{D})} &\leq N\|K'\delta\nu\psi\|_{C^0(\overline{D})} \\ &\leq N\|K'\|\,\|\psi\delta\nu\|_{2,\Omega} \end{aligned}$$

[as $K' : L^2(\Omega) \to C^0(\overline{D})$]

$$\leq N\|K'\|\,\|\psi\|_{C^0(\overline{\Omega})}\|\delta\nu\|_{2,\Omega} \;.$$

The quantity $\|\psi\|_{C^0(\overline{\Omega})} \leq \|\psi\|_{C^0(\overline{D})} \leq N\|\psi^i\|_{C^0(\overline{D})}$

from LEMMA 6.1 again.

This gives

$$\|\psi(\nu-\delta\nu) - \psi(\nu)\|_{C^0(\overline{D})} \leq N^2\|K'\|\,\|\psi^i\|_{C^0(\overline{D})}\|\delta\nu\|_{2,\Omega} \;.$$

The constant N depends upon $\|\nu-1\|_{2,\Omega}$ (as well as $\|K\|$ and $\|K'\|$). But as $\nu \in X_1$, $\|\nu-1\|_{2,\Omega} \leq M$ allowing us to make N independent of ν. Hence

$$\|\psi(\nu-\delta\nu) - \psi(\nu)\|_{C^0(\overline{D})} \leq N_0\|\delta\nu\|_{2,\Omega}$$

where N_0 is independent of ν as required. □

As Fréchet differentiability implies continuity, from THEOREM 6.2 we had continuity for $\nu \in L_2(\Omega)$ and $\|\nu-1\|_2 < 1/\|K\|$. To obtain Lipschitz continuity the stronger condition $\|\nu-1\|_2 \leq M < 1/\|K\|$ (where M is fixed) is required. That is the solution must belong to a bounded subset.

The method of proof in THEOREM 6.3 did not require the use of the implicit function theorem in contrast to the continuity/Fréchet differentiability result of THEOREM 6.2. This theorem could also have been arrived at via the mean value theorem for operators THEOREM 1.2 and the Fréchet differentiability result THEOREM 6.2 with

$$N_0 = \sup_{\nu \epsilon X_1} \|\psi'(\nu)\| \ .$$

We note our proof produces an explicit estimate for the Lipschitz constant N_0, that is

$$N_0 = N^2 \|K'\| \ \|\psi^i\|_{C^0(\overline{D})}$$

where

$$N = 1 + \frac{\|K'\| \ \|\nu-1\|_2}{1 - \|K\| \ \|\nu-1\|_2} \ .$$

6.3.4 *Compactness*

In this subsection we show the Fréchet derivative of the operator (6.1) (with continuous refractive indices) mapping into the space of continuous functions is compact. Thus the linearization of the operator in the case of point measurements of the field is compact.

The Fréchet derivative $U'(\nu)$ is given by (6.1) and (6.2). Using the approach suggested in §1.5.5 we have the following result.

THEOREM 6.4

The operator $U'(\nu) : C^0(\overline{\Omega}) \rightarrow C^0(\overline{D})$ with $\nu \ \epsilon \ X_0$, is compact.

<u>Proof</u> As $U : X_0 \rightarrow C(\overline{D})$ is Fréchet differentiable from THEOREM 6.1, $U'(\nu) : C^0(\overline{\Omega}) \rightarrow C^1(\overline{D})$ is a bounded linear operator for $\nu \ \epsilon \ X_0$. The imbedding $C^1(\overline{D}) \rightarrow C^0(\overline{D})$ is compact (Adams [1975] p.11). The result then follows from

the compactness of the composition of a compact and bounded operator (see THEOREM 1.3). □

We do not prove here the corresponding result for the nonlinear operator itself. This would require a boundedness result for the map $\nu \to \psi(\nu)$.

As the inverse of a compact linear operator is not bounded, we see that the solution of the linearized inverse problem with point measurements of the field is an ill-posed problem. We next investigate the application of regularization techniques which ensure the existence of a solution to both the linearized and nonlinear inverse problems.

6.3.5 *Regularization*

In addition to the problem of constructing solutions of the inverse problem, considered so far in this chapter, there is the question of the existence and stability of solutions in the presence of measurement noise. Then the measurement function

$$\Psi(\underline{x}) = \psi(\nu^*;\underline{x}) + \xi(\underline{x})$$

where ν^* is the actual coefficient function and $\xi(\underline{x})$ the noise. In this subsection the application of regularization techniques (see §1.3.2) to the inverse problem is investigated. Use is made of the Fréchet differentiability theorem just proved in formalizing these methods. We then relate our results to the numerical work of Roger *et al.* [1978].

Consider N different incident waves with measurements made at P points $\{\underline{x}_j\}$ along the measurement surface M. The operator equation to be solved is

$$U(\nu) = \psi_i(\nu;\underline{x}_j) - \Psi_i(\underline{x}_j) = 0 \ , \qquad i \in \{1,\dots,N\},\ j \in \{1,\dots,P\} \ .$$

We shall use the regularity theory obtained for continuous refractive indices.

To regularize the inverse problem the solution is restricted to lie within a suitable compact set. This is the Tikhonov selection method.

Consider the following problem

$$\text{minimize} \qquad \|U(\nu)\|^2 = \sum_{i,j} U_{ij}^{\,2}(\nu) \tag{6.22}$$

subject to $\nu \in X_3$,

where X_3 is a compact subset of $C^0(\overline{\Omega})$.

One possible choice for X_3 is

$$X_3 = \{\nu \in H^2(\Omega) : \|\nu\|_{H^2(\Omega)} \leq M \, , \, \nu \geq C > 0\} \ .$$

The constants M and C are given *a priori.* The compactness of X_3 follows from the compactness of the imbedding $H^2(\Omega) \rightarrow C^0(\overline{\Omega})$ in two or three dimensions (see the Sobolev imbedding theorem, Adams [1975] p.97). Note that if the refractive index is a function of only one variable, then $H^2(\Omega)$ may be replaced by $H^1(\Omega)$ in the above, as the imbedding $H^1(\Omega) \rightarrow C^0(\overline{\Omega})$ is then compact.

We then have the following result.

THEOREM 6.5

There exists a solution to the minimization problem (6.22).

<u>Proof</u> From THEOREM 6.1 the Fréchet differentiability of the operator equation (6.23) follows - this implies continuity also. The problem is then one of minimizing a continuous functional over a compact set for which there exists a solution (THEOREM 1.4). □

The numerical results of Roger *et al.* [1978] (and Roger [1978]) are interesting. They reconstruct one dimensional refractive indices using an iterative scheme. This scheme is derived in an ad hoc manner. However, like the Newton-Kantorovich method, it does require the solution of first kind integral equations.

A constraint of the form

$$\|\nu\|_{L^2(\Omega)} < M_1$$

was first applied. However, they found it necessary to replace this because of stability problems with

$$\|\nu\|_{H^1(\Omega)} < M_2$$

This is consistent with the need for the solution to belong to a compact subset in one dimension.

We do not prove a result for the continuous dependence of the solution of the regularized inverse problem upon the measurements, i.e., a stability result. However, a convergence result analogous to that of Colton and Kress [1983] p.238 could be proven (see §1.3.2).

Betero *et al.* have considered this question for the problem linearized about a constant initial approximation - that is within the Born approximation. They show the solutions of their regularized problem depend continuously upon the measurements. However, the continuity is only logarithmic in nature. This is much weaker than the Hölder continuity that may be obtained for some other inverse problems.

We note here that the linearized inverse problem (a compact operator equation from THEOREM 6.4) may also be formulated as a minimization problem analogous to (6.22) and an existence result like THEOREM 6.5 proven.

6.4 FAR-FIELD MEASUREMENTS

In this section the measurement of the far-field pattern rather than the field itself is considered. Consider an incident plane wave

$$\psi^{i}(\underline{x}) = \exp(i\underline{k}^{i}.\underline{x})$$

where the incident propagation vector

$$\underline{k}^{i} = k(\sin\theta^{i}\cos\varphi^{i}\underline{i} + \sin\theta^{i}\sin\varphi^{i}\underline{j} + \cos\theta^{i}\underline{k})$$

is in the direction given by the angular variables (θ^{i},φ^{i}) of the spherical polar coordinate system.

When $|\underline{x}| \rightarrow \infty$, the far-field behaviour is given by

$$\psi^{S}(\underline{x}) \sim \frac{\exp(ik|\underline{x}|)}{|\underline{x}|} g(\nu;\underline{k}^{i},\underline{k}^{S}) , \quad \underline{k}^{S} = \frac{k\underline{x}}{|\underline{x}|} \tag{6.23}$$

where the complex scattering amplitude $g(\nu;\underline{k}^{i},\underline{k}^{S})$ has the form

$$g(\nu;\underline{k}^{i},\underline{k}^{S}) = \frac{k^2}{4\pi} \int_{\Omega} \exp(-i\underline{k}^{S}.\underline{x}')[\nu(\underline{x}')-1]\, \psi(\underline{x}')dV' \ .$$

Here $\underline{k}^s$ is a vector of length k in the scattered direction represented by the angular variables (θ^s,φ^s), i.e.

$$\underline{k}^s = k(\sin\theta^s\cos\varphi^s\underline{i} + \sin\theta^s\sin\varphi^s\underline{j} + \cos\theta^s\underline{k}) \ .$$

6.4.1 *Newton–Kantorovich Method*

The nonlinear operator equation to be solved is

$$\breve{U}(\nu) = g(\nu;\underline{k}^i,\underline{k}^s) - G(\underline{k}^i,\underline{k}^s) = 0 \tag{6.24}$$

for a range of values of $\underline{k}^i$ and $\underline{k}^s$. The G are the measured values of $g(\nu^*)$, where ν^* is the true solution.

To derive the Fréchet derivative of $g(\nu)$ use is made of the following result from Weston [1980]

$$\begin{aligned} g(\nu_1;\underline{k}^i,\underline{k}^s) - g(\nu_2;\underline{k}^i,\underline{k}^s) \\ = \frac{k^2}{4\pi}\int_\Omega (\nu_1-\nu_2)\ \psi(\nu_2;\underline{k}^i)\ \psi(\nu_1;-\underline{k}^s)dV' \ , \end{aligned} \tag{6.25}$$

where $\psi(\nu;\underline{k})$ represents the total field produced by an incident wave in direction $\underline{k}$ upon a scatterer whose material properties are given by ν.

From (1.17) and (1.18)

$$g'(\nu)s = g(\nu+s) - g(\nu) + \epsilon(\nu;s)$$

where $$\lim_{||s||\to 0}\frac{||\epsilon(\nu;s)||}{||s||} = 0 \ ,$$

that is ϵ is a second order term in s.

Now

$$g(\nu+s) - g(\nu) = \frac{k^2}{4\pi}\int \psi(\nu;\underline{k}^i)\ \psi(\nu+s;-\underline{k}^s)s\ dV'$$

$$= \frac{k^2}{4\pi}\int \psi(\nu;\underline{k}^i)\ \psi(\nu;\underline{k}^s)s\ dV'$$

$$+ \frac{k^2}{4\pi}\int \psi(\nu;\underline{k}^i)[\psi(\nu+s;-\underline{k}^s) - \psi(\nu;-\underline{k}^s)]s\ dV'\ .$$

Then assuming this last term is of the second order (which will be proven later in §6.4)

$$g'(\nu)s = \frac{k^2}{4\pi}\int_\Omega \psi(\nu;\underline{k}^i)\ \psi(\nu;-\underline{k}^s)s\ dV'\ . \tag{6.26}$$

Then the equation for the update in the Newton-Kantorovich method with far-field measurements is

$$\breve{U}'(\nu^{(k)})s^{(k)} = -\breve{U}(\nu^{(k)})$$

or

$$\frac{k^2}{4\pi}\int_\Omega \psi(\nu^{(k)};\underline{k}^i)\ \psi(\nu^{(k)};-\underline{k}^s)s^{(k)}(\underline{x}')dV'$$

$$= G(\underline{k}^i,\underline{k}^s) - g(\nu^{(k)};\underline{k}^i,\underline{k}^s), \tag{6.27}$$

for a range of $\underline{k}^i$ and $\underline{k}^s$ values. This has an advantage over the Newton-Kantorovich method for measurement of field values alone - which was derived in the first section of this chapter. That is a Green function does not need to be computed for the kernel of the integral equation at each iteration.

6.4.2 *Born Approximation*

With an initial approximation $\nu^{(0)} = 1$ to the refractive index

$$\psi(1;\underline{k}^i) = \exp(i\underline{k}^i\cdot\underline{x}) ,$$

$$\psi(1;-\underline{k}^s) = \exp(-i\underline{k}^s\cdot\underline{x})$$

and $$g(1;\underline{k}^i,\underline{k}^s) = 0$$

From (6.27) the Born approximation applied to the inverse problem, with far-field measurements, is then

$$\frac{k^2}{4\pi}\int_\Omega \exp(i\underline{k}^i\cdot\underline{x}')\exp(-i\underline{k}^s\cdot\underline{x}')\, s^{(0)}(\underline{x}')\, dV' = G(\underline{k}^i,\underline{k}^s)$$

or

$$\int_\Omega \exp[i(\underline{k}^i-\underline{k}^s)\cdot\underline{x}']\, V(\underline{x}')dV' = 4\pi G(\underline{k}^i,\underline{k}^s) \tag{6.28}$$

where $$V(\underline{x}) = k^2 s^{(0)}(\underline{x})$$

is our approximate solution to the inverse problem.

Following Devaney [1978] we set $\underline{k}^i = k_0\underline{s}$ and $\underline{k}^s = k_0\underline{s}_0$, where $\underline{s}$ and $\underline{s}_0$ are unit vectors, and $k_0 = k$ is fixed. Then (6.28) becomes

$$\int_\Omega \exp[ik_0(\underline{s}-\underline{s}_0)\cdot\underline{x}']\, V(\underline{x}')dV' = 4\pi G(k_0\underline{s},k_0\underline{s}_0) \ . \tag{6.29}$$

Consider the threefold Fourier transform $\hat{V}(\underline{k})$ of $V(\underline{x})$

$$\hat{V}(\underline{k}) = \int_\Omega V(\underline{x}')\exp(-i\underline{k}\cdot\underline{x}')dV' \ . \tag{6.30}$$

On comparing (6.29) with (6.30) we conclude that

$$4\pi G(k_0\underline{s},k_0\underline{s}_0) = \hat{V}[k_0(\underline{s}-\underline{s}_0)] ,$$

which implies that the scattering amplitude determines $\hat{V}(\underline{k})$ for all those frequency vectors $\underline{k}$ given by

$$\underline{k} = k_0(\underline{s}-\underline{s}_0) \ . \tag{6.31}$$

For a given scattering experiment using an incident plane wave of fixed wave vector $k_0\underline{s}$ the values of $\underline{k}$ satisfying (6.31) lie on the surface defined by

$$\underline{k}\cdot\underline{k} = 2k_0^2(1-\underline{s}_0\cdot\underline{s}) \ .$$

It follows that if a (theoretically infinite) number of experiments were to be performed, all using incident plane waves of fixed wavenumber k_0 but varying directions of propagation $\underline{s}_0$, the totality of scattering data so obtained allows $\hat{V}(\underline{k})$ to be determined for all values of $\underline{k}$ lying within a sphere of radius $2k_0$. A band-limited approximation V_{b1} to V is then

$$V_{b1}(\underline{x}) = \frac{1}{(2\pi)^3} \int_{|\underline{k}| < 2k_0} \hat{V}(\underline{k}) \exp(i\underline{k}\cdot\underline{x})dV_k \tag{6.32}$$

where the Fourier amplitude is that which is reconstructed from the scattering amplitude.

If we assume that $V(\underline{x})$ is piecewise continuous and is localized within the finite volume Ω, its Fourier transform $\hat{V}(\underline{k})$ is an entire analytic function of the three Cartesian components k_x, k_y and k_z of the wave vector $\underline{k}$ (Plancheral-Polya theorem). It follows from analytic function theory that $\hat{V}(\underline{k})$ is uniquely determined for all values of $\underline{k}$ by its value within any finite volume element in $\underline{k}$ space. The extension of $\hat{V}(\underline{k})$ from its value over a finite volume element to all of $\underline{k}$ space can, in principle, be performed by analytic continuation. Because the set of scattering experiments described above yields $\hat{V}(\underset{\sim}{k})$ for all values of $\underset{\sim}{k}$ lying within the sphere $|\underset{\sim}{k}| < 2k$. The theorem just alluded to implies that $\hat{V}(\underset{\sim}{k})$ is completely determined for all values of $\underset{\sim}{k}$ by the scattering data. The complete reconstruction of $\hat{V}(\underset{\sim}{k})$ could, in principle, be performed using analytic continuation. However this is ill-conditioned for numerical computation and there are more practical ways of solving (6.29) for $V(\underset{\sim}{x})$. In particular a back propagation method for determining $V(\underset{\sim}{x})$ is outlined in Devaney [1982] and Devaney and Beylkin [1984]. This method has been implemented and some numerical results produced.

The update $s^{(k)}$ in the modified form of the Newton-Kantorovich method (with a unity initial approximation, i.e., $\nu^{(0)} = 1$) would satisfy

$$\breve{U}'(\nu^{(0)})s^{(k)} = -U(\nu^{(k)})$$

or

$$\frac{k^2}{4\pi}\int_{\Omega} \exp[i(\underset{\sim}{k}^i-\underset{\sim}{k}^s)\cdot\underset{\sim}{x}']\, s^{(k)}(\underset{\sim}{x}')dV'$$
$$= G(\underset{\sim}{k}^i,\underset{\sim}{k}^s) - g(\nu^{(k)};\underset{\sim}{k}^i,\underset{\sim}{k}^s)\,. \qquad (6.33)$$

Then the inversion of each iteration can be performed in the same manner as for the Born approximation - utilizing the band-limited approximation (6.32) or perhaps the back propagation method from Devaney [1982]. This modified Newton method may then be preferable to use than the scheme of Johnson and Tracy [1983] examined in §6.2. We note that such an approach has been applied to the corresponding inverse problem in geometric optics (see §7.3.2). There a filtered backprojection inversion is utilized at each iteration.

Such methods however are not valid in the low-frequency limit. It follows from §5.3 that the error in the Born approximation tends to zero as $k \to 0$. Several authors have utilized this fact (see Colton [1980] p.186 and Ramm [1983]) to devise reconstruction schemes in this low frequency limit. With these linear integral equations are obtained for the solution of the inverse problem. The methods utilize the analyticity in k of the scattering amplitude, for k small enough.

Colton considers the case where $V = V(r)$ is spherically symmetric. A moment problem for $m(r) = 1 - n^2(r)$ is obtained

$$\int_0^{r_0} m(r) r^{2n+2}\, dr = M_n \;, \; n = 0,1,2,\ldots \;.$$

The M_n are related to the limiting values (as $k \to 0$) of the far-field pattern.

We note this moment problem is of the same form as those derived in the Appendix for the linearization of the inverse problem considered there. Uniqueness of its solution in $L^2(0,r_0)$ would follow from the completeness of the $\{r^{2n+2}\}$.

6.4.3 *Fréchet Differentiability*

We now show that (6.26) is indeed the Fréchet derivative of the scattering amplitude. The result will be proven for a single value of $\underline{k}^i$ and $\underline{k}^s$, that is in (6.24) $\tilde{U} : X_0 \to \mathbb{R}$. The result then obviously extends to cover the case where measurements are available for a number of different values of $\underline{k}^i$ and $\underline{k}^s$. That is point measurements of the far-field are catered for. The proof makes use of the Fréchet differentiability result for a continuous refractive index derived in the previous section.

THEOREM 6.6

If $X_0 = \{\nu : \nu \in C^0(\overline{\Omega}),\ \nu > 0\}$ then the map $\nu \to g(\nu;\underline{k}^i,\underline{k}^s)$ from $X_0 \to \mathbb{R}$ is Fréchet differentiable with Fréchet derivative given by (6.26).

<u>Proof</u> From (6.25) and (6.26)

$$\epsilon(\nu;s) = g(\nu+s) - g(\nu) - g'(\nu)s$$

$$= \frac{k^2}{4\pi}\int_{\Omega} \psi(\nu;\underline{k}^i)[\psi(\nu+s;-\underline{k}^S) - \psi(\nu;-\underline{k}^S)]s \, dV' \quad .$$

So

$$|\epsilon(\nu;s)| \leq \frac{k^2}{4\pi} ||\psi(\nu;\underline{k}^i)||_{C^0(\overline{\Omega})} ||\psi(\nu+s;-\underline{k}^S) - \psi(\nu;-\underline{k}^S)||_{C^0(\overline{\Omega})} ||s||_{C^0(\overline{\Omega})} \int_{\Omega} dV' \ .$$

From the regularity result THEOREM 5.2

$$\begin{aligned} ||\psi(\nu;\underline{k}^i)||_{C^0(\overline{\Omega})} &\leq ||\psi(\nu;\underline{k}^i)||_{C^1(\overline{D})} \\ &\leq \eta_1 ||\psi^i||_{C^1(\overline{D})} \end{aligned}$$

giving

$$\begin{aligned} \frac{|\epsilon(\nu;s)|}{||s||_{C^0(\overline{\Omega})}} &\leq \eta_2 ||\psi(\nu+s;-\underline{k}^S) - \psi(\nu;-\underline{k}^S)||_{C^0(\overline{\Omega})} \\ &\leq \eta_2 ||\psi(\nu+s;-\underline{k}^S) - \psi(\nu;-\underline{k}^S)||_{C^1(\overline{D})} \quad . \end{aligned}$$

Now from THEOREM 6.1 $\psi(\nu)$ is Fréchet differentiable. This implies that $\psi(\nu)$ is continuous and

$$\lim_{||s|| \to 0} ||\psi(\nu+s) - \psi(\nu)||_{C^1(\overline{D})} = 0 \ .$$

Hence

$$\lim_{\|s\|\to 0} \frac{|\epsilon(\nu;s)|}{\|s\|_{C^0(\overline{\Omega})}} = 0$$

as required.

In addition, we need to check that $g'(\nu)$ is a bounded operator.

Now

$$g'(\nu)s = \frac{k^2}{4\pi}\int_\Omega \psi(\nu;\underline{k}^i)\ \psi(\nu;-\underline{k}^s)s\ dV'$$

so

$$|g'(\nu)s| \leq \frac{k^2}{4\pi}\|\psi(\nu;\underline{k}^i)\|_{C^0(\overline{\Omega})}\ \|\psi(\nu;-\underline{k}^s)\|_{C^0(\overline{\Omega})}\ \|s\|_{C^0(\overline{\Omega})}\int_\Omega dV'$$

$$\leq \frac{k^2}{4\pi}\|\psi(\nu;\underline{k}^i)\|_{C^1(D)}\ \|\psi(\nu;-\underline{k}^s)\|_{C^1(\overline{D})}\ \|s\|_{C^0(\overline{\Omega})}\int_\Omega dV'$$

$$\leq \eta_3\ \|s\|_{C^0(\overline{\Omega})}$$

and g' is bounded. □

A similar result making use of the Fréchet differentiability proof THEOREM 6.2 follows for refractive indices for which the Born series converges.

THEOREM 6.7

If $X_2 = \{\nu : \nu \in L^2(\Omega),\ \|\nu-1\|_{2,\Omega} < 1/\|K\|\}$ then the map $\nu \to g(\nu;\underline{k}^i,\underline{k}^s)$ from $X_0 \to \mathbb{R}$ is Fréchet differentiable with Fréchet derivative given by (6.26).

<u>Proof</u>

$$\epsilon(\nu;s) = \frac{k^2}{4\pi}\int_\Omega \psi(\nu;\underline{k}^i)[\psi(\nu+s;-\underline{k}^s) - \psi(\nu;-\underline{k}^s)]s\ dV' \ .$$

So

$$|\epsilon(\nu;s)| \leq \frac{k^2}{4\pi} ||\psi(\nu;\underline{k}^i)||_{C^0(\overline{\Omega})} ||\psi(\nu+s;-\underline{k}^S) - \psi(\nu;-\underline{k}^S)||_{C^0(\overline{\Omega})} \int_\Omega |s(\underline{x}')| \, dV' \ .$$

Using the Schwartz inequality

$$\int_\Omega |s(\underline{x}')| dV' = \int_\Omega |s(\underline{x}') \cdot 1| dV'$$

$$\leq ||s||_{L^2(\Omega)} \left[\int_\Omega dV' \right]^{\frac{1}{2}} \ .$$

From the regularity result THEOREM 5.4

$$||\psi(\nu;\underline{k}^i)||_{C^0(\Omega)} \leq \frac{||\psi^i||}{1 - ||K_\nu||} \ .$$

Hence $$\lim_{||s|| \to 0} \frac{|\epsilon(\nu;s)|}{||s||_{L^2(\Omega)}} = 0$$

follows from the continuity/Fréchet differentiability of $\psi(v)$ (THEOREM 6.2).

The boundedness of $g'(\nu)$ may then be established in a similar manner to THEOREM 6.6. □

COROLLARY 6.2

If $\nu = 1$, then

$$g'(\nu)s = \frac{k^2}{4\pi} \int_\Omega \exp(i\underline{k}^i \cdot \underline{x}') \exp(-i\underline{k}^S \cdot \underline{x}') \, s(\underline{x}') \, dV' \ ,$$

with $g'(1) : L^2(\Omega) \to \mathbb{R}$. □

This corollary shows that the Born approximation gives the formal linearization of the refractive index (squared) to far-field map, about a unity index.

6.4.4 *Completeness and Uniqueness*

We briefly outline here how the identity (6.25) and completeness arguments may be used to give uniqueness for the full nonlinear inverse problem at a single frequency. From (6.25)

$$g(\nu_1;\underset{\sim}{k}^i,\underset{\sim}{k}^S) - g(\nu_2;\underset{\sim}{k}^i,\underset{\sim}{k}^S) = \frac{k^2}{4\pi}\int_\Omega (\nu_1 - \nu_2)\ \psi(\nu_2;\underset{\sim}{k}^i)\ \psi(\nu_1;-\underset{\sim}{k}^S)\ dV' \ .$$

Ramm [1987] assumes the far-field $g(\nu;\underset{\sim}{k}^i,\underset{\sim}{k}^S)$ is known for all $\underset{\sim}{k}^i,\underset{\sim}{k}^S$ with $|\underset{\sim}{k}^i| = |\underset{\sim}{k}^S| = k$. So if

$$g(\nu_1;\underset{\sim}{k}^i,\underset{\sim}{k}^S) = g(\nu_2;\underset{\sim}{k}^i,\underset{\sim}{k}^S)$$

then

$$\int_\Omega (\nu_1 - \nu_2)\ \psi(\nu_2;\underset{\sim}{k}^i)\ \psi(\nu_1;-\underset{\sim}{k}^S)\ dV' = 0 \ .$$

He then establishes the completeness of the products of the solutions of the partial differential equation, i.e., the $\psi(\nu_1;-\underset{\sim}{k}^S)\ \psi(\nu_2;\underset{\sim}{k}^i)$. This gives $\nu_1 - \nu_2 = 0$ and uniqueness for $\nu \in L^\infty(\Omega)$.

We note this approach to uniqueness would also be applicable to the linearized inverse problem. If s_1 and s_2 are two solutions to the inverse problem linearized about ν, (6.27), then

$$\int_\Omega (s_1 - s_2)\ \psi(\nu;\underset{\sim}{k}^i)\ \psi(\nu;-\underset{\sim}{k}^S)\ dV' = 0 \ .$$

Completeness of the $\psi(\nu;\underline{k}^{i})\ \psi(\nu;-\underline{k}^{s})$ would give $s_1\text{-}s_2 = 0$ and uniqueness.

In addition completeness arguments can be used to give uniqueness of the solution of this inverse problem for the Helmholtz equation in the low frequency limit - see §6.4.2.

In a similar manner in the Appendix (Connolly and Wall [1988]) we obtain uniqueness of the linearized inverse problem of determining the conductivity in the steady-state diffusion equation from boundary measurements. There the corresponding integral relation

$$\int_{\Omega} (s_1\text{-}s_2)\ \nabla\phi(f;g_p) \cdot \nabla\phi(f;g_q)\ dV' = 0\ .$$

We established the completeness of the products $\nabla\phi(f;g_p) \cdot \nabla\phi(f;g_q)$ for f constant and the g_p,g_q belonging to a set of trigonometric boundary conditions, giving $s_1\text{-}s_2 = 0$ and uniqueness for this linearized case.

It can be shown that for the nonlinear version of that problem

$$\int_{\Omega} (f_1\text{-}f_2)\ \nabla\phi(f_1,g_p) \cdot \nabla\phi(f_2,g_q) = 0\ .$$

An extension of both our's and Ramm's arguments may then give uniqueness here for $f \in L^{\infty}(\Omega)$. We note here that Ramm has obtained uniqeness with $f \in W^{1,\infty}(\Omega)$ by utilizing a nonlinear transformation to the Helmholtz equation. Previous uniqueness arguments for the problem (Kohn and Vogelius [1985]) require piecewise analyticity of the coefficient function, although Kohn and Vogelius [1986] conjectured uniqueness for a much less smooth coefficient.

6.5 STEEPEST DESCENT

As an alternative to the Newton-Kantorovich method, several authors make use of the steepest descent and other gradient methods. Chavent [1973] and Kravaris and Seinfeld [1985] use gradient methods to solve the interior measurement problem we considered in Chapter Three. Lesselier [1984] uses the steepest descent method on a one-dimensional inverse scattering problem in the time-domain. Weston [1979, 1984] applies the method to the inverse scattering problem of this chapter.

In this section the steepest descent method is derived for our inverse scattering problem. We require the solution to belong to a Hilbert space (rather than $C^0(\overline{\Omega})$ as Weston does) as this simplifies things a little.

Before the steepest descent method (see Wouk [1979] pp.412-413) is outlined we first define the gradient of a functional. The gradient of J at v_0, denoted by $\nabla J(v_0)$, is an element of the Hilbert space X such that

$$J'(v_0)v = <\nabla J(v_0),v> \text{ , for all } v \in X . \tag{6.34}$$

$\nabla J(v_0)$ is uniquely defined from the Riesz representation theorem (Wouk [1979] pp.194-195).

The method of steepest descent to minimize J(v) is the following

$$v^{(n+1)} = v^{(n)} - t^{(n)}\nabla J(v^{(n)}) \ . \tag{6.35}$$

The $t^{(n)}$ are chosen to minimize J in the direction of steepest descent $-\nabla J(v^{(n)})$. That is $t^{(n)}$ is chosen such that

$$J(v^{(n)} - t^{(n)}\nabla J(v^{(n)})) \leq J(v^{(n)} - t^{(n)}\nabla J(v^{(n)})) \text{ , for all } t \ .$$

This requires a one-dimensional minimization at each step. We point out efficient procedures for this are available (e.g. various search techniques - see any standard text on optimization theory such as Fletcher [1980]).

6.5.1 *Inverse Problem Application*

The inverse problem with farfield measurements can be formulated as the problem of minimizing the following non-negative functional

$$J(\nu) = \Sigma|g(\nu;\underline{k}^i,\underline{k}^s) - G(\underline{k}^i,\underline{k}^s)|^2 \tag{6.36}$$

$$= \Sigma[g(\nu;\underline{k}^i,\underline{k}^s) - G(\underline{k}^i,\underline{k}^s)]\,\overline{[g(\nu;\underline{k}^i,\underline{k}^s) - G(\underline{k}^i,\underline{k}^s)]}$$

Here the summation is over all the different incident and scattered directions at which measurements are available.

We shall require $\nu \in L^2(\Omega)$ and be such that the Born series converges. To apply the steepest descent method we must be able to compute the gradient of $J(\nu)$.

$$J(\nu) = \Sigma(g(\nu) - G)\,\overline{(g(\nu) - G)}$$

so

$$\nabla J(\nu) = \Sigma[\overline{(g(\nu) - G)}\,\nabla g(\nu) + (g(\nu) - G)\,\overline{\nabla g(\nu)}]\ . \tag{6.37}$$

Thus the gradient $\nabla g(\nu)$ needs to be computed. From (6.26)

$$g'(\nu)s = \frac{k^2}{4\pi}\int_\Omega \psi(\nu;k^i)\,\psi(\nu;-k^s)s\,dV'$$

$$= \left\langle \frac{k^2}{4\pi}\psi(\nu;k^i)\,\psi(\nu;-k^s), s\right\rangle$$

so that

$$\nabla g(\nu) = \frac{k^2}{4\pi} \psi(\nu;-k^i)\ \psi(\nu;-k^s)\ . \tag{6.38}$$

To formalize this $g(\nu)$ must be Gateaux differentiable. This implied by the Fréchet differentiability of $g(\nu)$ which we have proven (THEOREM 6.7).

The steepest descent method (and similar schemes such as the conjugate gradient method) would be simpler to implement than the Newton-Kantorovich method. This is because (6.37) and (6.38) give an explicit formula for the update whereas the Newton method requires the solution of a linear operator equation at each iteration. Weston [1984] has obtained some numerical results for the reconstruction of a one-dimensional profile by minimizing a closely related functional to (6.36). However, nobody has yet applied gradient methods in two or more dimensions.

It should be noted that the order of convergence of the steepest descent method is not as good as Newton methods and their variants.

6.6 RICCATI WAVE EQUATION

The dependent variable transformation $\psi = \psi^i e^\phi$ applied to the Helmholtz equation may be used to obtain the following nonlinear equation

$$(\Delta+k^2)(\psi^i\phi) = -\ [\nabla\phi\cdot\nabla\phi + k^2(n^2-1)]\psi^i\ . \tag{6.39}$$

This can also be written in the form

$$\Delta\phi + \nabla\phi\cdot\nabla\phi + 2\nabla\ln\psi^i\cdot\nabla\phi + k^2(n^2-1) = 0\ . \tag{6.40}$$

The last equation is known as the Riccati wave equation. This particular form of the Helmholtz equation is of interest in certain situations that are explained later in the section.

The associated inverse problem is to determine the refractive index from a knowledge of ϕ.

Iterative methods have also been proposed to solve this inverse problem for (6.40) by Johnson *et al.* [1984]. The methods outlined are similar to those of Johnson and Tracy [1983] for the Helmholtz equation which were examined earlier in the chapter.

6.6.1 *Rytov Approximation*

An approximate method for solving the inverse problem for the Riccati equation analogous to the Born approximation for the Helmholtz equation may be derived. If the refractive index is near to unity, then $\psi \approx \psi^i$ and so $\phi \approx 0$. Neglecting the $\nabla\phi \cdot \nabla\phi$ term (which is of the second order in ϕ) gives

$$(\Delta + k^2)\,(\psi^i \phi) \approx -k^2(n^2-1)\psi^i \ .$$

Now $\psi^s = \psi^i(e^{\phi}-1) \simeq \psi^i\phi$ for $\phi \simeq 0$. Hence $\psi^i\phi$ satisfies the radiation condition for small ϕ.

And so
$$\psi^i\phi(\underline{x}) \approx \frac{k^2}{4\pi}\int_{\Omega} \frac{e^{ik|\underline{x}-\underline{x}'|}}{|\underline{x}-\underline{x}'|}[n^2(\underline{x}')-1]\;\psi^i(\underline{x}')\;dV' \tag{6.41}$$

giving

$$\phi(\underline{x}) \approx \frac{k^2}{4\pi}\int_{\Omega} \frac{e^{ik|\underline{x}-\underline{x}'|}}{|\underline{x}-\underline{x}'|}\;[n^2(\underline{x}')-1]\;\frac{\psi^i(\underline{x}')}{\psi^i(\underline{x})}dV' \ .$$

This approximate solution of the direct problem is known as the Rytov approximation (see Keller [1969]). Note that like the Born approximation, when applied to the inverse problem it gives a linear integral equation to solve for n^2 given ϕ.

Weston [1985] shows that (6.41) is in fact the first iterate in a convergent successive approximation scheme for ϕ. This is analogous to the Born approximation being the leading term in a Neumann series expansion for the field in the integral form of the Helmholtz equation. Alternatively Keller [1969] considered the Rytov approximation as the leading term of a formal asymptotic expansion.

Weston's expansion is for the following integral form of the equation (6.39)

$$\psi^i\phi(\underline{x}) = \int_\Omega \frac{1}{4\pi}\frac{e^{ik(\underline{x}-\underline{x}')}}{|\underline{x}-\underline{x}'|}[\nabla\phi(\underline{x}')\cdot\nabla\phi(\underline{x}') + k^2(n^2(\underline{x}')-1]\psi^i\, dV'$$

$$+ \text{ boundary integral terms.}$$

The boundary integral terms behave like ϕ^2 for small ϕ (and arise from the radiation condition).

Weston found the domain of convergence of the Rytov expansion to be greater than that for the Born series for a rapidly fluctuating medium. The two domains were similar for a slowly varying refractive index.

We have shown in §6.3 that the Born approximation applied to the inverse problem is actually the formal linearization (i.e. the Fréchet derivative) of the refractive index to field map. We now show the analogous result is true for the Rytov approximation.

Setting $\nu=n^2$, then $\phi(\nu)$ the corresponding map for the nonlinear form of the Helmholtz equation satisfies

$$\psi(\nu) = \psi^i e^{\phi(\nu)}$$

so that

$$\phi(\nu) \; = \ln\psi(\nu) - \ln\psi^{i}$$

and

$$\phi'(\nu)s = \frac{\psi'(\nu)s}{\psi(\nu)} \; .$$

This gives

$$\begin{aligned} \phi'(1)s \quad &= \frac{1}{\psi^{i}}\psi'(1)s \\ &= \frac{k^2}{4\pi}\int_{\Omega} \frac{e^{ik(\underline{x}-\underline{x}')}}{|\underline{x}-\underline{x}'|}\,\frac{\psi^{i}(\underline{x}')}{\psi^{i}(\underline{x})}s(\underline{x}')\,dV' \end{aligned} \tag{6.43}$$

from (6.2) (i.e. using the equivalent result for the Helmholtz equation).

Thus the Rytov approximation (6.41) when applied to the solution of the inverse problem is the linearization of $\phi(\nu)$ about a unity refractive index.

The Rytov approximation (6.41) for $\psi^{i}\phi$ is of the same form as the Born approximation for ψ. The single frequency techniques for the inverse problem discussed in §6.4 - the Fourier transform and filtered back propagation inversions - are then applicable. Devaney [1983] has numerically implemented his back propagation method within the Rytov approximation. We note these inversions could be extended to solve nonlinear problems with the modified form of the Newton-Kantorovich method - starting with an initial refractive index of unity.

At high frequencies the Rytov approximation is preferable to the Born approximation for the solution of the inverse problem. Devaney [1982] shows that as $k \rightarrow \infty$ inversion within the Rytov approximation reduces to conventional straight ray tomography (see Chapter Seven).

However there is still some argument over which of the Born and Rytov approximations is best to use and in what circumstances, for both the direct and inverse problems - see Leeman *et al.* [1985].

6.7 RELATED PROBLEMS

In this section we briefly consider two inverse problems closely related to the determination of a spatially varying refractive index in the Helmholtz equation. The first of these is the corresponding problem for vector generalizations of the Helmholtz equation. The second is an inverse problem in the time-domain for the wave equation.

6.7.1 *Vector Problems*

Two equations closely related to the scalar Helmholtz equation considered in previous chapters, are the linear elasticity equation and the vector Helmholtz equation. The solutions of both these equations are vector-valued rather than scalar-valued.

We first consider time-harmonic elastic waves in an isotropic body. The displacement at a point $\underset{\sim}{x}$ is $\underset{\sim}{u}(\underset{\sim}{x})$ with Cartesian components u_j and the stress tensor is τ_{jk}. The material occupying the body is of density ρ and its elastic properties are specified by the Lame parameters λ and μ. It will be assumed that there are no body forces. Then the equations to be satisfied are, when the time dependence is $e^{i\omega t}$

$$\tau_{jk} = \lambda \frac{\partial u_m}{\partial x_m} \delta_{jk} + \mu \left[\frac{\partial u_j}{\partial x_k} + \frac{\partial u_k}{\partial x_j}\right]$$

$$\frac{\partial \tau_{jk}}{\partial x_k} + \omega^2 \rho u_j = 0 , \tag{6.44}$$

respectively the constitutive equations for isotropic linear elasticity and Navier's equation. Here δ_{jk} is the standard Kronecker symbol and the usual summation convention has been employed. Eliminating the stress tensor gives (when λ and μ are constants)

$$\mu\Delta\underline{u} + (\lambda+\mu)\nabla(\nabla\cdot\underline{u}) + \omega^2\rho\underline{u} = 0 \ .$$

This can be written as

$$\frac{1}{k_{t^2}}\nabla x\nabla x\underline{u} + \frac{1}{k_\ell}\nabla\cdot(\nabla\cdot\underline{u}) + \omega^2\underline{u} = 0 \ . \tag{6.45}$$

The vector form of the Helmholtz equation is

$$\nabla x\nabla x\underline{u} - \omega^2 n^2\underline{u} = 0 \ . \tag{6.46}$$

The study of Maxwell's equations can be reduced to this equation. We note that if $\underline{u}$ has no longitudinal part, then (6.45) reduces to (6.46).

The associated inverse problem for the linear elasticity equation is to determine the possibly spatially-varying velocities of the longitudinal and transverse waves

$$c_\ell^2 = \frac{\lambda+2\mu}{\rho} \quad \text{and} \quad c_t^2 = \frac{\mu}{\rho} \ .$$

In the vector Helmholtz equation the spatially-varying n is to be determined as with the scalar equation.

Up till the present, most of the work done on these two inverse problems has utilized the Born approximation - see Cohen and Bleistein [1977]. Deriving a nonlinear operator theory for the solution of the inverse problems is more difficult than for the scalar Helmholtz equation. This is mainly due to the present lack of suitable regularity results. Uniqueness results for the direct problem with inhomogenous bodies have been proven by Jones [1982] and Wall [1988b] for the linear elasticity equation and for piecewise homogeneous bodies by Kupradze [1963]. However, we cannot use Fredholm alternative theory to obtain existence and regularity results from these as they stand, like we did for the Helmholtz equation. This is because the integral operators involved are not compact due to the presence of Green tensors with strong singularities. The Green function for the scalar Helmholtz equation has a weak singularity. As was stated in §5.4, pseudo-differential operator theory will then have a part to play with the Fredholm alternative theory being utilized.

We note here that existence and regularity results have been proven for Maxwell's equations in the quasi-static limit by Carey and O'Brien [1984]. These results are for piecewise constant constitutive parameters. They are motivated by practical applications in transient electromagnetic (TEM) prospecting.

6.7.2 *Time–domain Equations*

The linear acoustic wave equation with no losses is

$$\frac{1}{\rho c^2}\frac{\partial^2 u}{\partial t^2} - \nabla\cdot\left[\frac{1}{\rho}\nabla u\right] = 0 \tag{6.47}$$

subject to suitable initial and boundary conditions. The quantities $\rho, c \in \mathbb{R}$ are the spatially-varying density and sound velocity respectively. The inverse problem is to determine one or both of these quantities from measurements of the pressure u or its normal derivative on the surface of the region to be probed. We shall briefly review the work of several authors on this problem.

In a series of papers Symes [1983a, 1983b, 1986] examines the problem when c = constant, that is, ρ is to be reconstructed. Several theoretical results are proven - first the continuous dependence of the solution of the direct problem, u, upon the coefficient, ρ, is established. This is then extended to show that the map is indeed Fréchet differentiable. Then the stability of the linearized inverse problem is examined.

Fawcett [1985] considers the problem when ρ = constant, that is, c is to be found. A two-dimensional distribution is reconstructed using a Gauss-Newton type method - the Jacobian is computed using differences. To obtain these reconstructions one incident wave only is used, with measurements made in all directions over a period of time.

The special case of the inverse problem where the functions to be reconstructed are of one dimension only has been considered by many authors. This problem often arises in geophysical situations where the region is a stratified half-space. Most of the authors use direct (non-iterative) methods related to those of Gelfand and Levitan [1955] - see for example Krueger [1981] and Bube and Burridge [1983].

However, Bamberger *et al.* [1979] approach this one dimensional problem using operator methods - first establishing the continuity of the map between direct problem solution and the coefficient functions. Optimization (conjugate gradient) methods are then used to obtain numerical solutions.

Wall [1989] has examined the continuous dependence of the inverse problem solution upon the given data for a dissipative wave equation in the time domain. He utilizes explicit functional equations (obtained via invariant imbedding) for the mapping between the reflection kernel and the material functions to be identified. The non-dissipative case was examined in Vogel [1986].

For direct methods of determining the potential, $V(\underset{\sim}{x})$ in the plasma wave equation

$$\frac{\partial^2 u}{\partial t^2} - \Delta u - V(\underset{\sim}{x})u = 0 \ , \tag{6.48}$$

the reader is referred to Rose *et al.* [1984]. These methods are multidimensional - although not always economical for computation as the authors note.

The time-domain techniques of Rose *et al.* are closely related to multidimensional methods available for the Schrödinger equation in the frequency domain. These were derived by Newton [1980, 1981, 1982] and also Cheney [1984]. However, such direct methods require knowledge of the farfield at all frequencies. Also we are not aware of any numerical computations in more than one dimension. In contrast the nonlinear operator approach suggested in this chapter is applicable at a single frequency, plus the numerical implementation is relatively straightforward.

CHAPTER SEVEN

GEOMETRIC OPTICS

7.1 INTRODUCTION

With a large wavenumber it becomes necessary to use methods based upon geometric optics to solve the Helmholtz equation and its associated inverse problem. Then it becomes impossible to represent the field using conventional finite element methods (see §5.5).

It is therefore desired to construct a high-frequency asymptotic solution to the Helmholtz equation

$$[\Delta + k^2 n^2(\underline{x})]\,\psi(\underline{x}) = 0 \tag{7.1}$$

of the form

$$\psi(\underline{x}) \sim e^{ik\phi(\underline{x})} \sum_{m=0}^{\infty} \frac{\psi_m(\underline{x})}{(ik)^m} \ . \tag{7.2}$$

In this development $\psi_m(\underline{x})$ and $\phi(\underline{x})$ are assumed to be independent of the wavenumber k which is chosen as the large parameter.

Then as in Felson and Marcuwitz [1973], by substituting equation (7.2) into (7.1) and assuming that the differentiation can be performed on each term in the sum, one finds with $\bar{\underset{\sim}{k}} = \nabla\phi$

$$[(ik)^2(\bar{\underset{\sim}{k}}^2 - n^2) + (ik)(\nabla\cdot\bar{\underset{\sim}{k}} + 2\bar{\underset{\sim}{k}}\cdot\nabla) + \Delta] \sum_{m=0}^{\infty} \frac{\psi_m(\underline{x})}{(ik)^m} \sim 0 \ .$$

Since this expansion is to hold for arbitrary (though large) values of k, the coefficient of each power of k must vanish independently. From the k^2 term

$$|\bar{\underset{\sim}{k}}|^2 = n^2 \ , \tag{7.3}$$

from the k^1 term

$$(\nabla \cdot \bar{\underset{\sim}{k}} + 2\bar{\underset{\sim}{k}} \cdot \nabla)\psi_0 = 0 \ ; \tag{7.4}$$

and from the general term $k^{-\nu}$, $\nu = 0, 1, 2, \ldots$

$$\nabla \cdot \bar{\underset{\sim}{k}} + 2\bar{\underset{\sim}{k}} \cdot \nabla\psi_m = - \Delta\psi_{m-1} \, , \, m \geq 1 \, . \tag{7.5}$$

In deriving equations (7.4) and (7.5), the transport equations for the amplitude coefficients in the asymptotic expansion (7.2), use has been made of equation (7.3), the *eiconal equation* of geometrical optics. In view of the recursive character of the system of equations described by equation (7.5), all the coefficients ψ_m, $m > 1$, can be derived in principle from the lowest order coefficient ψ_0. The quantity ϕ is known as the phase function.

The lowest order solution of equation (7.2) in the high-frequency limit is the local plane-wave field

$$\psi \sim \psi_o e^{ik\phi} \ .$$

This "geometrical-optical" field dominates the remaining terms in (7.2) if the relative variation in the refractive index, $|\nabla n|/n$, is small compared with the local wavelength kn, i.e. if

$$\frac{|\nabla n|}{kn^2} << 1 \ . \tag{7.6}$$

If the medium is non-dissipative, so that n^2 is positive real, the procedure for solving the eiconal equation (7.3) involves determination of ray trajectories and then evaluating the phase function ϕ by integrating along a ray.

The rays are tangent to the ray vector $n\underset{\sim}{s} = \overline{\underset{\sim}{k}}$, where $\underset{\sim}{s}$ is a unit vector in the direction of $\overline{\underset{\sim}{k}}$ and perpendicular to the wavefront ϕ = constant.

The resulting ray equation is

$$\frac{d\underset{\sim}{r}}{ds} = \underset{\sim}{s} \, , \frac{d}{ds}(n\underset{\sim}{s}) = \nabla n \tag{7.7}$$

or $$\frac{d}{ds}\left[n\frac{d\underset{\sim}{r}}{ds}\right] = \nabla n \qquad \text{with} \qquad \left|\frac{d\underset{\sim}{r}}{ds}\right|^2 = 1 \, ,$$

where s denotes arc length.

In a homogeneous medium, for which n = constant, (7.7) has the solution

$$\underset{\sim}{r} = \underset{\sim}{A}s + \underset{\sim}{B}$$

where $\underset{\sim}{A}$ and $\underset{\sim}{B}$ are constant vectors. The rays in this case are straight lines. In an inhomogeneous medium where n varies continuously, the rays are smoothly curved. These rays bend towards a region of higher refractive index.

With ray trajectories computed from (7.7) we have for the phase function

$$\phi(\underset{\sim}{r}) - \phi(\underset{\sim}{r}_1) = \int_{\underset{\sim}{r}_1}^{\underset{\sim}{r}} n \, ds \, . \tag{7.8}$$

This phase integral defines the optical path length along the ray. In a homogeneous medium where n = constant and the rays are straight lines, one has

$$\phi(\underset{\sim}{r}) - \phi(\underset{\sim}{r}_1) = n|\underset{\sim}{r} - \underset{\sim}{r}_1| \ .$$

In a regular region where only one ray passes through a given point, it may be shown that for points $\underset{\sim}{r}_1$ and $\underset{\sim}{r}$ along a ray, the optical length in (7.8) is less along the ray than along any other neighbouring curve connecting the two points. This result is known as Fermat's principle.

We note that as the differential equations for the rays are nonlinear it is possible for several rays to pass through some point. The phase function is then multi-valued at such points. For a discussion of these difficulties and in particular the caustics that may result, the reader is referred to Jones [1986] §6.17 for example.

Finally a calculation in Felson and Marcuwitz [1973] shows that the amplitude is given by

$$|\psi_0(\underset{\sim}{r})| = |\psi_0(\underset{\sim}{r}_1)| \exp\left[-\tfrac{1}{2}\int_{\underset{\sim}{r}_1}^{\underset{\sim}{r}} \frac{1}{n}\nabla\cdot(n\underset{\sim}{s})ds\right] \tag{7.9}$$

where $n\underset{\sim}{s} = \nabla\phi$. We do not make any further use of this result, as the remainder of this chapter is concerned with the relationship between the refractive index and the phase function.

7.2 INVERSE PROBLEM

The inverse problem we will be concerned with is the determination of the refractive index, n, from knowledge of the phase function, ϕ. These two quantities are related by the eiconal equation (7.3)

$$|\nabla\phi|^2 = n^2 \ . \tag{7.10}$$

The main areas in which solving this inverse problem is of interest are in computer-assisted ultrasonic tomography, optical interferometry and exploration geophysics.

Consider the following configuration which has been utilized by several other authors. The rays travel from a transmitting plane at an angle θ to the x axis, through the object Ω inside which the refractive index n is spatially varying and then the measurements of ϕ, Φ, are made on an observing plane. The refractive index is equal to unity outside the object Ω and $\phi = 0$ on the transmitting plane.

This experiment is performed for a variety of angles θ_i to get sufficient information to be able to determine n. This requirement comes from conventional X-ray tomography, which is closely related to a linearized version of our inverse problem, as shall be seen later.

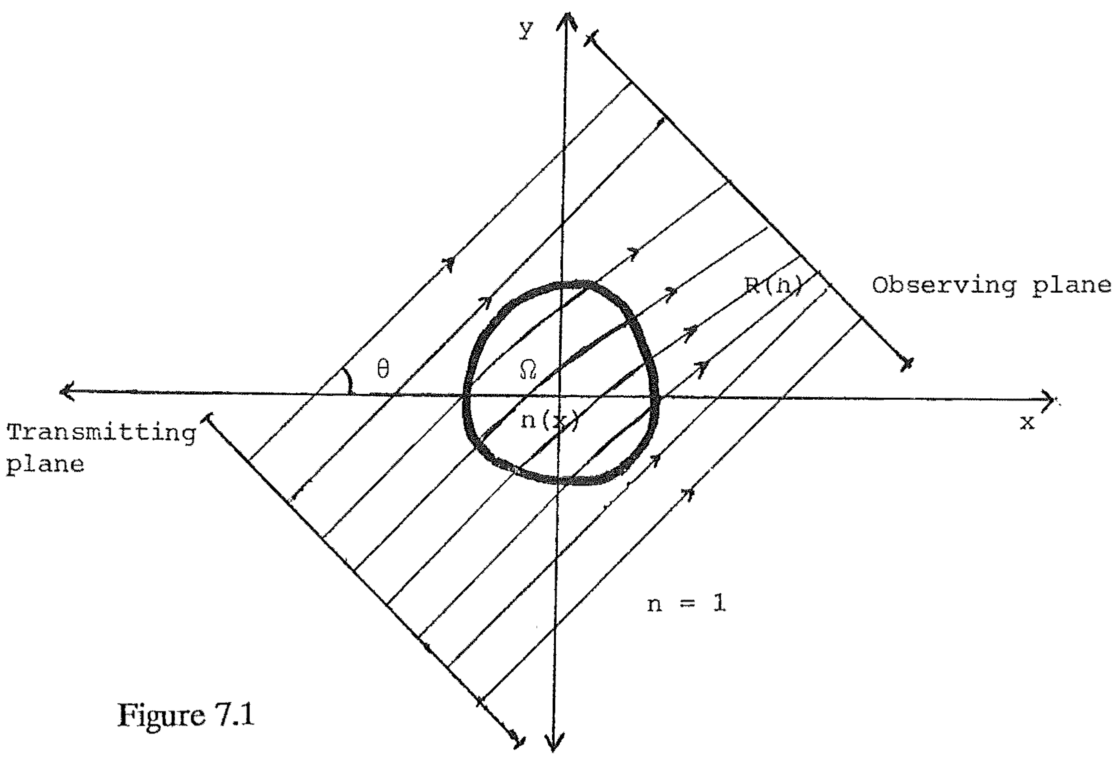

Figure 7.1

The measurements are made at a set of points $\{\underline{x}_j\}$ on the observing plane. The ray resulting from the refractive index n which passes through $\underline{x}_j$ is denoted by $R_j(n)$. To compute such a ray path a boundary value problem for a nonlinear second-order o.d.e. must be solved - see for example Lyttle and Dines [1980]. This differential equation is given by (7.7). The boundary value problem results are initially we know the angle the ray makes with the x-axis as well as its finishing point on the observation plane.

The alternative situation where the starting points of the rays are specified only requires the solution of initial value problems. This case is illustrated in Figure 7.1 where the rays are initially evenly spaced. However, such a situation does not occur as frequency in practical problems.

From the solution of the eiconal equation (7.8) we have

$$\Phi(\underline{x}_j) = \int_{R_j(n)} n(\underline{x}')ds_{\underline{x}'} \; . \tag{7.11}$$

Given the measurements $\Phi(\underline{x}_j)$ this is essentially a *nonlinear* integral equation for the refractive index n. The nonlinearity arises as the ray paths over which the integrals are made, depend upon n.

7.2.1 *Straight Ray Approximation*

To solve the inverse problem several authors - Glover and Sharp [1977] and Mueller *et al* [1979] for example, use what is known as the straight ray approximation. In this the rays $R_j(n)$ above are approximated by straight rays R_j (which result when the refractive index n = 1 inside Ω) in (7.11).

Then

$$\Phi(\underline{x}_j) = \int_{R_j} n(\underline{x}')\, ds_{\underline{x}'} \; . \tag{7.12}$$

When $\underline{x}_j$ is varied along points of the observing plane, and the experiment is performed for a number of different incident directions θ_i (7.12) becomes a *linear* integral equation to be solved for n. This same problem of inverting (7.12) arises in X-ray computed tomography - see Bates and Peters [1971] for example.

There are two possible approaches to solving (7.12). The first is the algebraic method where it is discretized using a collocation type approach (see Anderson and Kak [1984]). That is n is expressed as a basis function expansion and measurements are taken at a set of points $\{\underline{x}_j\}$ for a set of incident angles $\{\theta_i\}$. This gives a linear system of algebraic equations to be solved. The system is sparse in nature and there are special methods of solution available.

Secondly, there exist analytic solutions of (7.12). These are based upon either Fourier transform techniques or a filtered back projection of the measured values (see Davison and Grunbaum [1981]). These methods are cheaper to utilize than the algebraic method (and are usually used in a practical implementation) however they are not as flexible. For example, they cannot be generalized to handle curved rays which the algebraic method obviously can.

7.2.2 *Iterative Methods*

The straight ray approximation has been extended into an iterative method by Lyttle and Dines [1980]. For the first iteration the straight path approximation is used giving an initial approximation $n^{(1)}$ to the refractive index. Then the rays resulting from the refractive index $n^{(1)}$ are computed. The rays $R_j(n)$ in (7.11) are then approximated by the rays $R_j(n^{(1)})$ and the equation is solved for a new approximate solution $n^{(2)}$. This scheme is then repeated in an iterative manner.

That is

$$\Phi(\underset{\sim}{x}_j) = \int_{R_j(n^{(k)})} n^{(k+1)}(\underset{\sim}{x}')ds_{\underset{\sim}{x}'}, \tag{7.13}$$

is the linear equation to be solved for $n^{(k+1)}$ at each iteration. The algebraic method of solution described in §7.2.1 is used to solve this equation.

With their iterative technique Lyttle and Dines obtain significant improvements over straight ray reconstructions for the same problems. Schomberg [1978] uses a similar iterative scheme, however the improvements obtained are not as marked. This is probably because the refractive index he reconstructs is fairly close to unity - $\max_{\Omega} |n - 1| = 0.05$ c.f. 0.3 for Lyttle and Dines.

To compute each ray path the two-point boundary value problem for a second order ordinary differential equation resulting from (7.7) must be solved. The equation is nonlinear and shooting-type methods may be used. Keller and Perozzi [1983] solve the resulting nonlinear system of equations using Newton's method. It should be noted that this is applying Newton's method to the solution of the nonlinear direct problem rather than the inverse problem, to which we apply the Newton-Kantorovich method in the next section.

We also note that for some refractive indices there may be several different rays passing through a given point - resulting in a multivalued solution. This is due to the nonlinear nature of the direct problem. Authors encountering this situation generally only consider the shortest path ray to a measurement point. However, we are of the opinion that in this case all possible ray paths to the point should be utilized. This is because McKinnon and Bates [1980] point out that a shortest path ray may not travel through regions around a local maximum in the refractive index. To use all the ray paths the scheme for solving the direct problem must be capable of finding all the solutions of the two-point boundary value problem.

We also note here that geometric optics ideas may usefully be incorporated into solutions of both the direct and inverse problems for the Helmholtz equation proper - see for example Tan and Bates [1988] and Bates [1989].

7.3 NEWTON-KANTOROVICH METHOD

In this section the Newton-Kantorovich method is derived in an informal manner. The Fréchet differentiability of this problem is formalized in §7.3.3.

Consider one set of incident rays parallel to the x-axis with measurements $\Phi(y)$ performed on the line $x = a$.

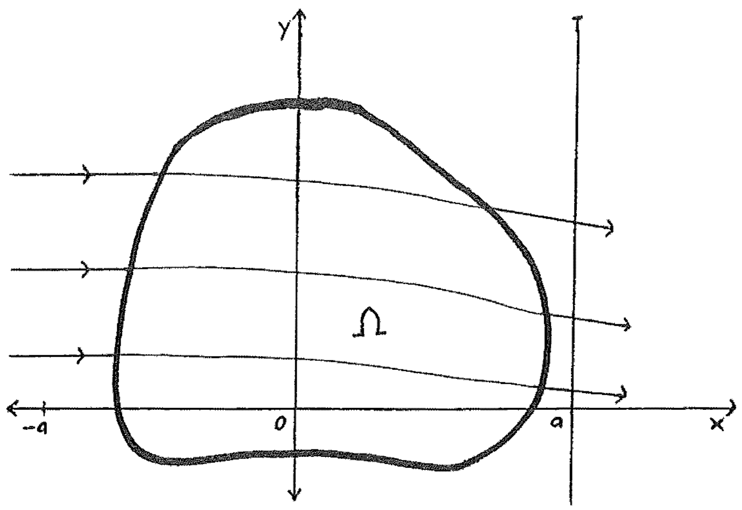

Figure 7.2

Our methods may then easily be modified to cover a number of sets of incident rays at varying angles to the x-axis.

7.3.1 *Derivation*

The operator equation to be solved is

$$V(n) = \phi(n;a,y) - \Phi(y) = 0 \ .$$

The Fréchet differential of V (assuming it exists) is then

$$V'(n)t = \phi'(n)t\big|_{x = a} \ .$$

Again the Fréchet derivative of the direct problem solution, $\phi'(n)$ must be computed. We use the approach suggested in §1.4.2.

Differentiating the direct problem formulation

$$\nabla\phi(n)\cdot\nabla\phi(n) = n^2 \ , \quad \phi = 0 \quad \text{when} \quad x = -a \tag{7.14}$$

with respect to n gives

$$2\nabla\phi'(n)t \cdot \nabla\phi(n) = 2nt \ , \quad \phi'(n)t = 0 \ \text{ when } \ x = -a$$

so that

$$\nabla\phi'(n)t \cdot \nabla\phi(n) = nt \ . \tag{7.15}$$

This last equation is a first order linear hyperbolic equation for $\phi'(n)t$ (as $\nabla\phi(n)$ is known), which has characteristics given by

$$\begin{aligned} \frac{d\underset{\sim}{r}}{ds} &= \frac{\nabla\phi}{|\nabla\phi|} \\ &= \frac{\nabla\phi}{n} \end{aligned} \tag{7.16}$$

from using (7.14). Now $n\underset{\sim}{s} = \nabla\phi$ and so

$$\frac{d\underset{\sim}{r}}{ds} = \underset{\sim}{s} \ .$$

Hence the characteristics of this linear equation are the same as the rays (7.7) for the nonlinear equation (7.14).

Along these characteristics (7.15) reduces to the ordinary differential equation

$$|\nabla\phi(n)|\frac{d\phi'}{ds}(n)t = nt$$

giving

$$\phi'(n)t\Big|_{\underset{\sim}{x} = \underset{\sim}{P}} = \phi'(n)t\Big|_{\underset{\sim}{x} = \underset{\sim}{Q}} + \int \frac{nt}{|\nabla\phi|} ds$$

where the integral is over the characteristic between $\underset{\sim}{P}$ and $\underset{\sim}{Q}$. But $|\nabla\phi| = n$ and also if we specify $\underset{\sim}{Q}$ to be on $x = -a$ then

$$\phi'(n)t = \int_{R(n)} t \ ds$$

as the characteristics are also the rays.

So the update $t^{(k+1)}$ in the Newton-Kantorovich method satisfies

$$\int_{R(n^{(k)})} t^{(k+1)}(\underset{\sim}{x}') \, ds_{\underset{\sim}{x}'} = \Phi(y) - \phi(n^{(k)}; a,y) \quad . \tag{7.17}$$

But

$$\int_{R(n^{(k)})} n^{(k)}(\underset{\sim}{x}')ds_{\underset{\sim}{x}'} = \phi(n^{(k)})$$

and

$$t^{(n+1)} = n^{(k+1)} - n^{(k)}.$$

Hence

$$\int_{R(n^{(k)})} n^{(k+1)}(\underset{\sim}{x}')ds_{\underset{\sim}{x}'} = \Phi(y) \tag{7.18}$$

is the linear equation to be solved for the new approximation $n^{(k+1)}$.

Note however this is the same equation as (7.13) which is used by Lyttle and Dines [1980] in their iterative scheme (which they derived in a fairly ad hoc manner).

The solution of the eiconal equation, ϕ, may be multi-valued, i.e., there may exist more than one ray to a point $\underset{\sim}{x}_j$. Then similarly the Fréchet differential $\phi'(n)t$ is multi-valued, and all these rays should be considered in Newton's method.

Fawcett and Keller [1985] have also applied Newton's method to a geophysical problem of this type. However, their refractive index is layered and piecewise constant, with these constants and the shape of the interfaces to be determined. Due to this special form for the refractive index they use an alternative method to compute their Jacobian/Fréchet derivative.

7.3.2 *Modified Newton Method*

In addition consider the linearization about an approximation $n^{(0)}$ = constant. Then the rays are straight i.e., $R_{n^{(0)}} = R$ and $\phi(n^{(0)}; \underset{\sim}{x}) = c\ (x + a)$ giving

$$\int_R t^{(1)} (\underset{\sim}{x}')ds_{\underset{\sim}{x}'} = \Phi(y) - 2ca$$

or equivalently

$$\int_R n^{(1)}(\underline{x}')ds_{\underline{x}'} = \Phi(y) \ .$$

From (7.12) this equation is the same as that which results from the straight ray approximation. That is conventional tomographic techniques result from the linearization of our operator about a constant refractive index. In a similar manner we saw in §6.4.2 that Devaney's diffraction tomography arose from the linearization of the corresponding map for the Helmholtz equation about a constant refractive index.

Of particular interest is the modified form of the Newton-Kantorovich method (see (1.13)). If a constant refractive index is chosen as the initial approximation $n^{(0)}$, then as was just noted, the rays $R_{n^{(0)}} = R$ are straight. The update $t^{(k+1)}$ in the iterative scheme satisfies

$$\int_R t^{(k+1)}(\underline{x}')ds_{\underline{x}'} = \Phi(y) - \phi(n^{(k)}; a,y) \ . \qquad (7.19)$$

This has the advantage that analytic methods of solution can be utilized. That is, the filtered back projection method or Fourier transform techniques can be used to solve the linear operator equation at each iteration.

Iteration schemes of this form have been used by McKinnon and Bates [1980] for a problem in ultrasonic tomography and Cha and Vest [1981] for a problem in optical interferometry. Again the schemes were derived in an ad hoc manner.

McKinnon and Bates (see also McKinnon [1980]) reconstruct radially symmetric distributions. However, the improvement over the straight ray reconstructions is not marked as only a small perturbation on a constant distribution is considered - when the straight ray approximation can be expected to be fairly accurate.

Cha and Vest reconstruct both axisymmetric and asymmetric two dimensional refractive index distributions and obtain significant improvements over the straight ray reconstructions. This is because they reconstruct distributions with a reasonable variation from a constant distribution.

We note that when the modified form of the Newton-Kantorovich method is used it is not necessary to compute a new set of ray paths at each iteration - instead a finite difference technique (such as that of Bates and McKinnon) may be used to solve the direct problems.

7.3.3 *Fréchet Differentiability*

In this subsection we briefly examine the Fréchet differentiability of the map $n \to \phi(n)$. Regularity theory for the direct problem is scarce - probably due to its nonlinearity. The only result in this direction we are aware of is due to Bloom and Kazarinoff [1976]. They show that if n belongs to C^2 and is close enough to unity, i.e. $\sup[|n - 1|, |\text{grad } n|]$ is small enough then existence and uniqueness for the solution to the eiconal equation follows. This is proven by using a fixed point theorem for contractions applied to an integral form of the ray equations.

Laurentiev *et al.* [1970] have shown that (7.17) is in fact the linearization of the operator equation. They use the form (7.11) for the direct problem and utilize Fermat's theorem.

So from their work the error in the linearization is of the second order for a refractive index, $n \in C^2$. This regularity requirement is implied by the ray equations. This also assumes the existence of a solution to the eiconal equation. As the Fréchet derivative is bounded for $n \in C^2$ (this follows from our THEOREM 7.1 (i) in the next section) we have that Fréchet differentiability of the map $n \to \phi(n)$ follows.

We also note that Oliker [1987] proves Fréchet differentiability when considering a linearized version of an inverse reflection problem from geometric optics. We have been considering an inverse refraction problem. He notes that Newton's method would then be applicable to his problem.

7.4 REGULARIZATION

In addition to the problem of constructing solutions of the inverse problem considered in the previous sections, there is the question of the existence and stability of these solutions, particularly in the presence of measurement noise. In this section we examine the application of regularization techniques to the solution of the linear problem (7.18). This is then related to the numerical work of Lyttle and Dines [1980]. The regularization of the fully nonlinear inverse problem is not considered, but would require stronger constraints on the refractive index.

Instabilities are present in the solution of the inverse problem. Evidence of this is in the need to differentiate measurement data in Fourier reconstruction methods for the straight ray problem. Also Anderson and Kak [1984] obtain noise in their numerical results with the algebraic reconstruction method. Our results shall also cover curved ray inversions.

Consider M different sets of incident rays giving the measurement functions $\{\Phi_i(\underline{x})\}$. The measurements are made at N points $\{\underline{x}_j\}$ along the observation plane.

The linearized operator equation to be solved is then

$$\tilde{V}_{ij}(n^{(k+1)}) = \int_{R_{ij}(n^{(k)})} n^{(k+1)} ds - \Phi_i(\underline{x}_j) = 0 , \qquad (7.2)$$

$$i \epsilon \{1,...,M\},\ j \epsilon \{1,...,N\} .$$

$R_{ij}(n^{(k)})$ is the ray arriving at $\underline{x}_j$ in the ith set of incident rays, resulting from the refractive index $n^{(k)}$. Note the equation (7.20) is a linear operator equation as the rays $R_{ij}(n^{(k)})$ are known.

To regularize the linear inverse problem the solution is restricted to lie within a suitable compact set - see §1.3.2 and §1.5.5.

Consider the following problem

$$\text{minimize } \|\tilde{V}(n^{(k+1)})\|^2 = \sum_{i,j} \tilde{V}_{ij}^2(n^{(k+1)}) \tag{7.21}$$

subject to $n^{(k+1)} \in X_0$,

where X_0 is a compact subset of $C^0(\Omega)$. We shall show that $\tilde{V}$ is a continuous operator on $C^0(\Omega)$.

One possible choice for X_0 is

$$X_0 = \{n \in H^2(\Omega) \ : \ \|n\|_{H^2(\Omega)} \leq M\} \ . \tag{7.22}$$

The compactness of X_0 follows from the compactness of the imbedding $H^2(\Omega) \to L^\infty(\Omega)$ in two or three dimensions (see the Sobolev imbedding theorem, Adams [1975] p.97).

This choice is particularly appropriate for numerical applications where Hilbert spaces are generally used. Note that if the refractive index is a function of only one dimension, then $H^2(\Omega)$ may be replaced by $H^1(\Omega)$ in the above, as the imbedding $H^1(\Omega) \to L^\infty(\Omega)$ is then compact.

We then have the following result

THEOREM 7.1 (i) $\tilde{V} : C^0(L) \to \mathbb{R}^{nxm}$ is a bounded operator.

(ii) There exists a solution to the minimization problem (7.21).

<u>Proof</u>

(i) $$\tilde{V}_{ij}(n+t) - \tilde{V}_{ij}(n) = \int_{R_{ij}} t \, ds$$

giving

$$|\tilde{V}_{ij}(n+t) - \tilde{V}_{ij}(n)| \leq ||t||_{\infty,\Omega} \cdot (\text{length of ray})$$

and

$$||\tilde{V}(n+t) - \tilde{V}(n)|| \leq (MN)^{\frac{1}{2}} \cdot (\text{length of longest ray}) \cdot ||t||_{\infty,\Omega}$$

and so $\tilde{V}$ is bounded.

(ii) The problem then becomes one of minimizing a continuous functional over a compact set - to which there exists a solution from Theorem 1.4. □

It has just been shown that the measurements depend continuously upon the function to be reconstructed and that there exists a solution of the regularized linear inverse problem.

This then gives some theoretical justification to the work of Lyttle and Dines [1980]. They add a smoothness constraint of the form

$$||\nabla^2 n||_2 \leq M_1$$

which they call a Laplace filter. It should be noted (see Gustafson [1980] p.170 for example) that the space with norm

$$||u||^2 = ||u||_2^2 + ||\nabla u||_2^2 + ||\nabla^2 u||_2^2$$

is equivalent to $H^2(\Omega)$, and that our theorem holds for the constraint

$$||n||_{H^2(\Omega)} \leq M .$$

We do not prove a result for the continuous dependence of solutions of the regularized problem upon the measurements. However, Betero *et al.* [1979] have examined this stability question in the straight ray case, where an analytic solution is available. They consider square integrable refractive indices, i.e. $n \in L^2(\Omega)$ and also a square integrable measurement function $\Phi(\underline{x})$.

A constraint of the form

$$\left[\frac{\partial n}{\partial x}\right]^2 + \left[\frac{\partial n}{\partial y}\right]^2 \leq M_2$$

(the problem is in two dimensions) is imposed on the derivatives of the refractive index. They they show that the reconstructed function depends Hölder continuously upon the measurement function. This continuity is stronger than the logarithmic continuity obtained for the inverse problem for the Helmholtz equation at one frequency within the Born approximation.

We note as their result is for a square integrable measurement function it would not be applicable to the point measurements utilized in Theorem 7.1. There a stronger constraint (on the second rather than first derivatives) is required.

The reader is also referred to Davison and Grunbaum [1981] who apply regularization methods similar to those of Backus and Gilbert [1970] to the tomographic (straight ray) problem.

CHAPTER EIGHT

CONCLUSIONS

8.1 SUMMARY

In Chapter One we provided a general framework for solving a wide class of inverse problems. The inverse problem is formulated as a nonlinear operator equation. This may be solved by the Newton-Kantorovich iterative method and its variants. Existence and stability of solutions in the presence of measurement noise may be obtained by using regularization techniques. The continuity and Fréchet differentiability of the nonlinear operator can be examined by means of the implicit function theorem. Methods for showing the boundedness or compactness of the operator were also discussed.

In Chapter Three an inverse problem for steady-state diffusion was considered. Some properties of the direct problem were outlined in Chapter Two. The inverse problem was formulated as a nonlinear operator equation. We then derived the Newton-Kantorovich method for solution of the equation. This is a new approach to this particular problem - most of the work on this problem to date being performed in finite dimensional spaces. The Gauss-Newton method for parameter identification was also derived and its relationship with the Newton-Kantorovich method outlined. We produced some numerical results for a one-dimensional problem and used regularization techniques in the presence of measurement noise.

Finally the Fréchet differentiability of the nonlinear operator considered in this chapter was proven. Boundedness, Lipschitz continuity and compactness results were also obtained and the theoretical application of regularization techniques investigated.

Chapter Four was concerned with the inverse boundary scattering problem. First uniqueness and continuous dependence results for the inverse problem and existing methods for its solution were reviewed. We then extended a previous continuous dependence result for the farfield upon the boundary shape - removing the requirement for the solution to belong to a compact set. The use of the Newton-Kantorovich method combined with the null-field method of solution for the direct problem was outlined. In addition, the partial differential equation satisfied by the Fréchet differential was derived and the relationship of the Fréchet derivative with the Hadamard variation examined. Finally, we investigated determining an unknown impedance boundary condition from farfield measurements and a Fréchet differentiability result was proven for this problem.

In Chapter Six we considered the determination of a spatially varying refractive index in the Helmholtz equation. The properties of the direct problem were outlined in Chapter Five - including some new regularity theory in Sobolev spaces. The inverse problem was formulated as a nonlinear operator equation in Chapter Six. The Newton-Kantorovich method for the solution of the equation was then derived. We found that the two dimensional reconstruction technique of Johnson and Tracy is closely related to the method we propose.

Two new Fréchet differentiability results were proven in the chapter. The first was for continuous refractive indices within the regularity theory provided by Fredholm's theorem. The second was for a square integrable coefficient within the regularity theory given by the Born series and Banach's theorem. These results are then used in the regularization of the inverse problem.

We also found that the Fréchet derivative for farfield measurements is particularly simple - not involving a Green's function but just the field alone. This was formalized using the Fréchet differentiability results just outlined. We then examined the Born approximation and also the method of steepest descent.

Finally we considered the Rytov approximation for the Riccati form of the wave equation and also possible extensions of our work to vector generalizations of the Helmholtz equation.

Chapter Seven was concerned with an inverse problem from geometric optics. We outlined the use of the straight line approximation and also iterative methods for its solution. Existing iterative schemes were shown to be forms of the Newton-Kantorovich method. A regularization result for the linearized inverse problem was also proven.

In the Appendix the determination of the electrical conductivity of an object (from knowledge of both the potential and normal current) on its boundary is examined. The inverse problem was again formulated as a nonlinear operator equation and the Fréchet derivative computed. For our choice of operator the derivative did not involve the calculation of Green's functions. This then gave a moment problem to solve at each iteration of the Newton-Kantorovich method.

Some questions of a theoretical nature were then examined. First the nonlinear moment operator was shown to be Fréchet differentiable, i.e. we had formally linearized it. The result was then used in regularizing the problem, where continuity of the operator is required - this being implied by differentiability.

The linearization of the inverse problem about a constant conductivity on a circle was also considered. An analytic expression for the Fréchet derivative is obtained in this case and a uniqueness result for the linearized inverse problem proven. We then utilized the analytic form for the derivative to reconstruct radially symmetric conductivities with the modified Newton-Kantorovich method. Some numerical results were presented.

8.2 CONCLUSIONS

We shall now outline some of the main points that arise from the work of this thesis. Firstly, some of the advantages of using the nonlinear operator methods advocated are outlined. The approach is applicable to a variety of inverse problems, for any type of differential equation and in any number of spatial dimensions. As well as determining a spatially varying coefficient in a differential equation, the Newton-Kantorovich method and its variants may be used to solve inverse boundary scattering problems as was seen in Chapter Four.

The approach extends approximate methods of solution, such as the Born approximation for the problem of Chapter Six, into algorithms providing solutions to the full nonlinear problem. Regularization methods giving the existence and stability of solutions in the presence of measurement noise may be incorporated.

Nonlinear operator methods may be used to reconstruct functions which are not very smooth. Evidence of this is provided by our numerical results in the Appendix in which discontinuous functions were reconstructed. All that is required is a suitable regularity result, allowing us to prove Fréchet differentiability. The Newton-Kantorovich method may then be applied. Other methods for solving inverse problems often require fairly strong smoothness assumptions on the function to be reconstructed.

Importantly for many inverse problems, at present it seems there is no other way of reconstructing an arbitrary function, apart from formulating the problem as a nonlinear operator equation and using iterative methods of solution. That is, no direct (non-iterative) method of solution exists as yet. Examples of such inverse problems are the two or three dimensional electrical conductivity imaging problem and determining a refractive index in the Helmholtz equation at one frequency.

Another important point that arises out of our work is the need to examine theoretical questions in addition to a numerical solution of the inverse problem. There are numerous iterative schemes for the solution of inverse problems in the literature which have been derived in an ad hoc manner. Many of these upon further investigation turn out to be variants of the Newton-Kantorovich method (or perhaps gradient methods). Some authors derive what they call Newton methods but neglect to prove Fréchet differentiability. Such knowledge gives us an idea of how the iterative scheme can be expected to behave, and how we may go about improving its performance. In addition, many approximate methods for the solution of inverse problems are obtained in an ad hoc manner. These often may be formalized as the linearization of our nonlinear operator equation about some simple approximation (such as a constant function).

Many authors also apply regularization methods in an informal manner. They formulate the problem as a minimization of a functional and constraints are added. But they do not prove continuity for the functional nor compactness of the set over which the minimization takes place. Without such results we cannot be sure that there exists a stable solution to the regularized problem.

Indeed, we were able to show that smoothness constraints seemingly pulled out of the air by several authors were in fact consistent with the solution belonging to a compact set. We imagine these constraints were arrived at by trial and error whereas a generally applicable approach to finding them is given in this thesis.

Other authors treat the problem as one of parameter identification - discretizing the problem at the start and using the Gauss-Newton method for example, to solve the resulting system of nonlinear algebraic equations. We take the view that it is in general preferable to formulate the problem as a nonlinear operator equation, then discretizing to obtain numerical solutions. This is because we would rather examine the properties of the operator equation in an infinite dimensional setting than in a finite dimensional space after discretizing it. It should be noted that the same equations are obtained whether we first linearize the problem and then discretize or we first discretize and then linearize.

8.3 FUTURE RESEARCH

We give a number of areas in which future research relating to the work of this thesis is warranted.

(1) More extensive *numerical testing* of the algorithms we have derived for our inverse problems (and also for inverse problems in general) would be useful. A number of authors, including ourselves, have successfully reconstructed functions of one dimension.
Work has been done on reconstructing two or three dimensional functions but more is required here.

(2) The question of *uniqueness* has not been resolved for a number of different inverse problems. In addition it may be possible to reduce the smoothness requirements in uniqueness results already available - for example, the boundary measurement problem of the Appendix.

(3) Even less is known about the *characterisation* of solutions to inverse problems. The limited amount of literature available on this problem is mainly confined to inverse scattering and even this does not completely answer such questions.

(4) Results for the *stabilization* of nonlinear inverse problems are also scarce. That is, proofs for the stability of regularized inverse problems are required. A number of linearized inverse problems have been investigated in this regard, however not much is known in the nonlinear cases.

(5) *Convergence* results for iteration schemes (such as the Newton-Kantorovich method) applied to inverse problems would be useful. General results are available from optimization theory, and these should be applicable to the solution of the problems of this thesis and others.

(6) More investigation of *properties* such as continuity and Fréchet differentiability is required for the nonlinear operator equation formulation of some inverse problems. These properties are needed to produce algorithms for solving the inverse problem.

With our work and that of other authors several results are available for the steady-state diffusion equation and also refractive index and boundary scattering problems for the Helmholtz equation. Results have also been proven for the time-domain diffusion and wave equations with spatially varying coefficients and also the boundary scattering problem for the Helmholtz equation. However, there are a number of important problems for which such results are not available. For example, the Riccati wave equation and the vector-valued generalizations of the Helmholtz equation considered earlier are in this category. A Fréchet differentiability result is also required for our operator formulation of inverse boundary scattering - only continuity has been shown at present.

In addition, there is a need to reduce the smoothness requirements for the results already proven. For instance, the results available for the boundary scattering problem of the Helmholtz equation require a continuously differentiable surface and there is interest in reducing this requirement. Also, our Fréchet differentiability result for the Helmholtz equation with spatially varying refractive index requires this index to be continuous. A result applicable to discontinuous indices would also be of interest.

(7) Further development of existence, uniqueness and *regularity theory* is required for the direct problems in which there is much interest in solving the corresponding inverse problem. Again, such results are required for geometric optics, the Riccati wave equation and boundary and refractive index scattering problems for vector forms of the Helmholtz equation. We can then utilize these results to establish the properties of the nonlinear operator defining the inverse problem.

REFERENCES

Adams [1975] R.A. Adams. *Sobolev Spaces.* Academic Press, New York, 1975.

Alessandrini [1988] G. Alessandrini. Stable determination of conductivity by boundary measurements. *Applicable Analysis,* 27 : 1453-172, 1988.

Anderson and Kak [1984] A.H. Anderson and A.C. Kak. Simultaneous algebraic reconstruction technique (SART) : A superior implementation of the ART algorithm. *Ultrasonic Imaging,* 6(1): 81-94, January 1984.

Anderssen [1975] R.S. Anderssen. On the inversion of global electromagnetic induction data. *Physics of the Earth and Planetary Interiors,* 10: 292-298, 1975.

Anderssen [1980] R.S. Anderssen. On the use of linear functionals for Abel-type integral equations. In R.S. Anderssen, F.R. de Hoog and M.A. Lukas, editors, *The Application and Numerical Solution of Integral Equations.* Sijthoff and Nordhoff, Alphen and den Rijn, 1980.

Anderssen and Dietrich [1987] R.S. Anderssen and C.R. Dietrich. *The Inverse Problem of Aquifer Transmissivity Identification.* Research Report, Centre for Mathematical Analysis, The Australian National University, Canberra, 1987.

Angell *et al.* [1982] T.S. Angell, D. Colton and A. Kirsch. The three dimensional inverse scattering problem for acoustic waves. *Journal of Differential Equations,* 46 : 46-58, 1982.

Angell *et al.* [1987] T.S. Angell, R.E. Kleinmann and G.F. Roach. An inverse transmission problem for the Helmholtz equation. *Inverse Problems,* 3(2) : 149-180, May 1987.

Astley [1983] R.J. Astley. Wave envelope and infinite elements for acoustical radiation. *International Journal for Numerical Methods in Fluids,* 3 : 507-526, 1983.

Astley and Eversman [1983] R.J. Astley and W. Eversman. Finite element formulations for acoustical radiation. *Journal of Sound and Vibration,* 88(1) : 47-64, 1983.

Babuska and Aziz [1972] I. Babuska and A.K. Aziz. Survey lectures on the mathematical foundations of the finite element method. In A.K. Aziz, editor, *The Mathematical Foundations of the Finite Element Method with Applications to Partial Differential Equations,* pp.3-362, Academic Press, New York, 1972.

Backus and Gilbert [1967] G.E. Backus and J.F. Gilbert. Numerical applications for a formalism for geophysical inverse problems, *Geophysical Journal of the Royal Astronomical Society,* 13 : 247-276, 1967.

Backus and Gilbert [1970] G.E. Backus and J.F. Gilbert. Uniqueness in the inversion of inaccurate gross earth data. *Philosophical Transactions of the Royal Society of London, Series A : Mathematical and Physical Sciences,* A266 : 123-192, March 197

Baker [1977] C.T.H. Baker. *The Numerical Treatment of Integral Equations.* Clarendon Press, Oxford, 1977.

Bamberger *et al.* [1979] A. Bamberger, G. Chavent and P. Lailly. About the stability of the inverse problem in 1-D wave equations - application to the interpretation of seismic profiles. *Applied Mathematics and Optimization,* 5(1) : 1-47, 1979.

Bates [1984] R.H.T. Bates. Full-wave computed tomography. Part 1 : Fundamental theory. *IEE Proceedings Part A,* A131(8) : 610-61 November 1989.

Bates [1989] R.H.T. Bates. WKB/Rayleigh-Gans (Born) inverse scattering approximation and reconstruction algorithm. *Inverse Problems,* 4 : L29-L32, 1988.

Bates and McDonnell [1986] R.H.T. Bates and M.J. McDonnell. *Image Restoration and Reconstruction. Oxford engineering science series volume 16.* Clarendon Press, Oxford, 1986.

Bates and Peters [1971] R.H.T. Bates and T.M. Peters. Towards improvements in tomography. *New Zealand Journal of Science,* 14(4) : 883-900, December 1971.

Bates and Tan [1985] R.H.T. Bates and D.G.H. Tan. Towards reconstructing phases of inverse-scattering signals. *Journal of the Optical Socie of America A,* 2(11) : 2013-2018, November 1985. Special Issue on Inverse Problems in Propagation and Scattering.

Bates and Wall [1976] R.H.T. Bates and D.J.N. Wall. Chandrasekhar transformations improve convergence of computations of scattering from linearly stratified media. *IEEE Transactions on Antennas and Propagation,* AP24(2) : 251-253, March 1976.

Bates and Wall [1977] R.H.T. Bates and D.J.N. Wall. Null field approach to scalar diffraction : I. General Method. *Philosophical Transactions of the Royal Society of London, Series A : Mathematical and Physical Sciences, A287(133a).* A287(1339) : 45-78, September 1977.

Betero *et al.* [1979] M. Betero, C. De Mol and G.A. Viano. The stability of inverse problems. In H.P. Baltes, editor, *Inverse Scattering Problems in Optics,* pp.161-124, Springer-Verlag, Berlin, 1979.

Bloom and Kazarinoff [1976] C.O. Bloom and N.D. Kazarinoff. *Short Wave Problems in Inhomogenous Media : Asymtotic Solutions. Lectur Notes in Mathematics, Volume 522.* Springer-Verlag, Berlin, 1976.

Boerner *et al.* [1981] W.M. Boerner, A.K. Jordan and I.W. Kay. Introduction to the special issue on inverse methods in electromagnetics, *IEEE Transactions on Antennas and Propagation,* AP-29(2) : 185-189, 1981

Breckon and Pidcock [1987] W.R. Breckon and M.K. Pidcock. Mathematical aspects of impedance imaging. *Clinical Physics and Physiological Measurement*, 8 (Supplement A) : 77-84, 1987.

Bube and Burridge [1983] K.P. Bube and R. Burridge. The one-dimensional inverse problem of reflection seismology. *SIAM Review*, 25(4) : 497-559, October 1983.

Calderon [1980] A.P. Calderon. On an inverse boundary value problem. *Seminar on Numerical Analysis and its applications to Continuum Mechanics.* Soc. Brasilera de Matematica, Rio de Janeiro, pp.65-73, 1980.

Carey and O'Brien [1984] A.L. Carey and D.M. O'Brien. *Existence and Regularity Results for Maxwell's Equations in the Quasi–static Limit.* Research Report No. 50, Department of Mathematics, Australian National University, Canberra, 1984.

Cha and Vest [1981] Soyoung Cha and C.M. Vest. Tomographic reconstruction of strongly refracting fields and its application to interferometric measurement of boundary layers. *Applied Optics*, 20(16) : 2787-2794, August 1981.

Chadan and Sabatier [1977] K. Chadan and P.C. Sabatier. *Inverse Problems in Quantum Scattering Theory. Texts and Monographs in Physics.* Springer-Verlag, New York, 1977.

Chavent [1973] G. Chavent. Identification of distributed parameters. In P. Eykhoff, editor. *Proceedings of the 3rd IFAC Symposium*, North-Holland, Amsterdam, 1973.

Chen and Mei [1975] H.S. Chen and C.C. Mei. Hybrid element for water waves. *Proceedings of the Modelling Techniques Conference*, (*Modelling 1975*), *San Francisco, 3–5 September 1975*, 1 : 63-81.

Chen [1979] Y.M. Chen. An iterative procedure for solving inverse scattering problems arising from remote sensing. In J.A. De Santo *et al.*, editors, *Mathematical Methods and Applications of Scattering Theory, Lecture Notes in Physics 130*, pp.308-310, Springer-Verlag, Berlin, 1979.

Chen and Liu [1981] Y.M. Chen and J.Q. Liu. A numerical algorithm for remote sensing of thermal conductivity. *Journal of Computational Physics*, 43 : 315-326, 1981.

Chen and Liu [1982] Y.M. Chen and J.Q. Liu. A numerical algorithm for solving inverse problems of two-dimensional wave equations. *Journal of Computational Physics*, 50 : 193-208, 1982.

Chen and Tsien [1977] Y.M. Chen and D.S. Tsien. A numerical algorithm for remote sensing of density profiles of a simple ocean model by acoustic pulses. *Journal of Computational Physics*, 25 : 366-385, 1977.

Cheney [1984] M. Cheney. Inverse scattering in dimension two. *Journal of Mathematical Physics*, 25(1) : 99-107, January 1984.

Coen *et al.* [1981] S. Coen, K.K. Mei and D.J. Angelakos. Inverse scattering technique applied to remote sensing of layered media. *IEEE Transactions on Antennas and Propagation*, 29(2) : 298-306, March 1981.

Coen and Yu [1981] S. Coen and M.W-H Yu. The inverse problem of the direct current conductivity profile of a layered earth. *Geophysics*, 46(12) : 1702-1713, December 1981.

Cohen and Bleistein [1977] J.K. Cohen and N. Bleistein. An inverse method for determining small variations in propagation speed. *SIAM Journal of Applied Mathematics*, 32 : 784-799, 1977.

Colton [1980] D. Colton. *Analytic Theory of Partial Differential Equations.* Pitman, London, 1980.

Colton [1984] D. Colton. The inverse scattering problem for time-harmonic acoustic waves. *SIAM Review*, 26 : 323-350, 1984.

Colton and Kirsch [1981a] D. Colton and A. Kirsch. Stable methods for solving the inverse scattering problem for a cylinder. *Proceedings of th Royal Society of Edinburgh*, 89A : 181-188, 1981.

Colton and Kirsch [1981b] D. Colton and A. Kirsch. The determination of the surface impedance of an obstacle from the measurements of the far-field pattern. *SIAM Journal on Applied Mathematics*, 41 : 8-15, 1981.

Colton and Kress [1983] D. Colton and R. Kress. *Integral Equation Methods in Scattering Theory*, John Wiley, New York, 1983.

Colton and Monk [1985] D. Colton and P. Monk. A novel method for solving th inverse scattering problem for time-harmonic acoustic waves in t resonance region. *SIAM Journal on Applied Mathematics*, 45(6) : 1039-1052, December 1985.

Colton and Monk [1986] D. Colton and P. Monk. A novel method for solving th inverse scattering problem for time-harmonic acoustic waves in t resonance region II. *SIAM Journal on Applied Mathematics*, 46 506-523, 1986.

Colton and Monk [1987] D. Colton and P. Monk. The inverse problem for time-harmonic acoustic waves in a penetrable medium. *Quarter Journal of Mechanics and Applied Mathematics*, 40(2) : 184-212, May 1987.

Colton and Monk [1988] D. Colton and P. Monk. The inverse scattering problem for time-harmonic acoustic waves in an inhomogenous medium. *Quarterly Journal of Mechanics and Applied Mathematics*, 4(1) 97-125, February 1988.

Colton and Sleeman [1983] D. Colton and B.D. Sleeman. Uniqueness theorems for the inverse problem of acoustic scattering. *IMA Journal of Applied Mathematics*, 31 : 253-259, 1983.

Connolly [1985] T.J. Connolly. *Inverse Problems for an Elliptic Equation.* Master's thesis, Department of Mathematics, Unviersity of Canterbury, Christchurch, New Zealand, 1985.

Connolly and Wall [1988] T.J. Connolly and D.J.N. Wall. On an inverse problem, with boundary measurements, for the steady state diffusion equation. *Inverse Problems*, 4 : 995-1012, 1988.

Connolly *et al* [1985] T.J. Connolly, D.J.N. Wall and R.H.T. Bates. Inverse problems and the Newton-Kantorovich method. In A.J. Devaney and R.H.T. Bates, editors, *Inverse Optics II*, pages 30-34, August 1985. Proceedings SPIE volume 558 (the Society of Photo-Optical Instrumentation Engineers).

Costabel and Stephan [1987] M. Costabel and E.P. Stephan. Coupling of finite elements and boundary elements for transmission problems of elastic waves in $\mathbb{R}^3$. *Proceedings of UTAM Conference, San Antonio, USA*, 1987.

Courant and Hilbert [1962] R. Courant and D. Hilbert. *Methods of Mathematical Physics, Volume 2*, Interscience, New York.

Daniel [1971] J.W. Daniel, *The Approximate Minimization of Functionals.* Prentice-Hall, Englewood Cliffs, New Jersey, 1971.

Davison and Grunbaum [1981] M.E. Davison and F.R. Grunbaum. Tomographic reconstruction with arbitrary directions. *Communications on Pure and Applied Mathematics*, 34 : 77-120, 1981.

Devaney [1978] A.J. Devaney. Nonuniqueness in the inverse scattering problem. *Journal of Mathematical Physics*, 19(7) : 1526-1531, July 1978.

Devaney [1982] A.J. Devaney. A filtered backpropagation algorithm for diffraction tomography. *Ultrasonic Imaging*, 4(4) : 336-350, October 1982.

Devaney [1983] A.J. Devaney. A computer simulation of diffraction tomography. *IEEE Transactions on Biomedical Engineering*, BME-30(7) : 377-386, July 1983. Special Issue on Medical Ultrasound.

Devaney and Beylkin [1984] A.J. Devaney and G. Beylkin. Diffraction tomography using arbitrary transmitter and receiver surfaces. *Ultrasonic Imaging*, 6(2) : 181-193, April 1984.

Devaney and Wolf [1982] A.J. Devaney and E. Wolf. A new perturbation expansion for inverse scattering from three-dimensional finite-range potentials. *Physics Letters*, 89A(6) : 269-272, May 1982.

Dietrich *et al.* [1988] C.R. Dietrich, G.N. Newsam, R.S. Andersson, A.J. Jakeman and F. Ghassemi. *A Practical Account of Instabilities in Identification Problems in Groundwater Systems.* Research Report, p.29-88, Centre for Mathematical Analysis, The Australian National University, Canberra, 1988.

Elden [1988] Lars Elden. *Algorithms for the Computation of Functionals Defined or the Solution of a Discrete Ill–posed Problem.* Research Report, Centre for Mathematical Analysis, The Australian National University, Canberra, 1988.

Falk [1983] R.S. Falk. Error estimates for the numerical identification of a variable coefficient. *Mathematics of Computation*, 40(162) : 537-546, April 1983.

Fawcett [1985] John Fawcett. Two dimensional velocity inversion of the acoustic wave equation. *Wave Motion*, 7 : 503-513, 1985.

Fawcett and Keller [1985] John Fawcett and H.B. Keller. Three dimensional ray tracing and geophysical inversion in layered media. *SIAM Journal on Applied Mathematics*, 45(3) : 491-500, June 1985.

Felsen and Marcuwitz [1973] L.B. Felsen and N. Marcuwitz. *Radiation and Scattering of Waves*, Englewood Cliffs, New Jersey, 1973.

Fienup [1978] J.R. Fienup. Reconstruction of an object from the modulus of its Fourier transform. *Optics Letters*, 3(1) : 27-29, July 1978.

Fletcher [1980] R. Fletcher. *Practical Methods of Optimization*, *Vol. 1, Unconstrained Optimization.* Wiley, Chichester, 1980.

Friedman and Gustafsson [1987] A. Friedman and B. Gustafsson. Identification o the conductivity coefficient in an elliptic equation. *SIAM Journ on Mathematical Analysis*, 18(3) : 777-787, May 1987.

Frind and Pinder [1973] E.O. Frind and G.F. Pinder. Galerkin solution of the inverse problem for aquifer transmissivity. *Water Resources Research*, 9(5) : 1397-1410, October 1973.

Garabedian [1955] P.R. Garabedian. An integral equation governing electromagnetic waves. *Quarterly on Applied Mathematics*, 12 : 428-433, 1955.

Garabedian [1964] P.R. Garabedian. *Partial Differential Equations.* Wiley, New York, 1964.

Gelfand and Levitan [1955] I.M. Gelfand and B.M. Levitan. On the Determination of a Differential Equation from its Spectral Function. *American Mathematical Society Translations, Series 2* 1 : 253-304, 1955.

Gilbarg and Trudinger [1977] D. Gilbarg and H.S. Trudinger. *Elliptic Partial Differential Equations of the Second Order.* Springer, New York, 1977.

Glover and Sharp [1977] G.H. Glover and J.C. Sharp. Reconstruction of ultrasound propagation speed in soft tissue: Time-of-flight tomography. *IEEE Transactions on Sonics and Ultrasonics*, SU-24(4) : 229-234, July 1977.

Golub and Kahan [1965] G.H. Golub and W. Kahan. Calculating the singular values and pseudo-inverse of a matrix. *SIAM Journal of Numerical Analysis*, 2 : 202-224, 1965.

Gray and Hagin [1982] S.M. Gray and F. Hagin. Towards precise solution of one-dimensional velocity inverse problems. *SIAM Journal on Applied Mathematics*, 42(2) : 346-355, April 1982.

Gustafson [1980] K.E. Gustafson. *Introduction to Partial Differential Equations and Hilbert Space Methods.* John Wiley, New York, 1980.

Hanson [1971] R.J. Hanson. A numerical method for solving Fredholm integral equations of the first kind using singular values. *SIAM Journal on Numerical Analysis*, 8(3) : 616-622, September 1971.

Hatcher and Chen [1983] R.P. Hatcher and Y.M. Chen. An iterative method for solving inverse problems of a nonlinear wave equation. *SIAM Journal on Scientific and Statistical Computing*, 4(2) : 149-163, June 1983.

Hutson and Pym [1980] V. Hutson and J.S. Pym. *Applications of Functional Analysis and Operator Theory.* Academic Press, London, 1980.

John [1978] F. John. *Partial Differential Equations.* Springer-Verlag, New York, third edition, 1978.

Johnson and Tracy [1983] S.A. Johnson and M.L. Tracy. Inverse scattering solutions by a sinc basis, multiple source, moment method - Part 1 : Theory. *Ultrasonic Imaging*, 5(4) : 361-375, October 1983.

Johnson *et al.* [1984] S.A. Johnson, Y. Zhou, M.L. Tracy, M.J. Berggren, and F. Stenger. Inverse scattering solutions by a sinc basis, multiple source, moment method - Part III : Fast algorithms. *Ultrasonic Imaging*, 6(1) : 103-116, January 1984.

Jones [1984a] D.S. Jones. A uniqueness theorem in elastodynamics. *Quarterly Journal on Mechanics and Applied Mathematics*, 37 : 121-142, 1984.

Jones [1984b] D.S. Jones. An exterior problem in elastodynamics. *Mathematical Proceedings of the Cambridge Philosophical Society*, 96 : 173-182, 1984.

Jones [1985] D.S. Jones. Note on a uniqueness theorem of Schiffer. *Applicable Analysis*, 19 : 181-188, 1985.

Jones [1986] D.S. Jones. *Methods in Electromagnetic Wave Propagation*, Clarendon Press, Oxford, 1986.

Jost and Kohn [1952] R. Jost and W. Kohn. Construction of a potential from a phase shift. *The Physical Review*, 87(6) : 977-994, 1952.

Keller [1969] J.B. Keller. Accuracy and validity of the Born and Rytov approximations. *Journal of the Optical Society of America*, 59(8) : 1003-1004, August 1969.

Keller and Perozzi [1983] H.B. Keller and D.J. Perozzi. Fast seismic ray tracing *SIAM Journal on Applied Mathematics*, 43 : 981-992, 1983.

Kittappa and Kleinmann [1975] R. Kittappa and R.E. Kleinmann. Acoustic scattering by penetrable homogenous objects. *Journal of Mathematical Physics*, 16 : 421-432, 1975.

Kleinmann and Martin [1987] R.E. Kleinmann and P.A. Martin. On single integ equations for the transmission problem of acoustics. *SIAM Journal on Applied Mathematics*, 48 : 307-325, 1987.

Kohn and Vogelius [1984] R.V. Kohn and M. Vogelius. Determining conductivi by boundary measurements. *Communications on Pure and Applied Mathematics*, 37 : 289-298, 1984.

Kohn and Vogelius [1985] R.V. Kohn and M. Vogelius. Determining conductivi by boundary measurements II. Interior results. *Communicatio on Pure and Applied Mathematics*, 38 : 643-667, 1985.

Kohn and Vogelius [1987] R.V. Kohn and M. Vogelius. Relaxation of a variational method for impedance computed tomography. *Communications on Pure and Applied Mathematics*, 40 : 745-777, 1987.

Kravaris and Seinfeld [1985] C. Kravaris and J.H. Seinfeld. Identification of parameters in distrubuted parameter systgems by regularization. *SIAM Journal on Control and Optimization*, 23(2) : 217-241, *March 1985.*

Kress and Roach [1978] R. Kress and G.F. Roach. Transmission problems for th Helmholtz equation. *Journal of Mathematical Physics*, 19 : 1433-1437, 1978.

Kristensson and Vogel [1986] G. Kristensson and C.R. Vogel. Inverse problems for acoustic waves using the penalised likelihood method. *Inver Problems*, 2(4) : 461-479, November 1986.

Krueger [1982] R.J. Krueger. Inverse problems for nonabsorbing media with discontinuous material properties. *Journal of Mathematical Physics*, 23(3) : 396-404, 1982.

Kupradze [1963] V.D. Kupradze. *Progress in Solid Mechanics, Vol. 3.* North-Holland, Amsterdam, 1963.

Laurentiev *et al.* [1970] M.M. Laurentiev, V.G. Romanov and V.G. Vasiliev. *Multidimensional Inverse Problems for Differential Equations.* Springer, New York, 1970.

Lax and Phillips [1967] P.D. Lax and R.S. Phillips. *Scattering Theory. Pure and Applied Mathematics, a series of monographs and textbooks ; volume 26.* Academic Press, New York, 1967.

Lee and Seinfeld [1987] T. Lee and J.H. Seinfeld. Estimation of absolute and relative permeabilities in petroleum reservoirs. *Inverse Problems* 3(4) : 711-728, 1987

Leeman *et al.* [1985] S. Leeman, M.A. Fiddy and L. Zapalowski. Born versus Rytov : is the debate over? In A.J. Devaney and R.H.T. Bates, editors. *Inverse Optics II*, pages 11-14, August 1985. Proceedings SPIE volume 558 (the Society of Photo-Optical Instrumentation Engineers).

Leis [1967] R. Leis. *Vorlesungen uber Partielle Differential–Gleichungen Zweiter Ordnung.* Bibliographisches Institut, Mannheim, 1967.

Lesselier [1982] D. Lesselier. Optimization techniques and inverse problems : reconstruction of conductivity profiles in the time domain. *IEEE Transactions on Antennas and Propagation*, AP-30(1), January 1982.

Linz [1979] P. Linz. *Theoretical Numerical Analysis.* Wiley-Interscience, New York, 1979.

Lyttle and Dines [1980] R.J. Lyttle and K.A. Dines. Iterative ray-tracing between boreholes for underground image reconstruction. *IEEE Transactions on Geoscience and Remote Sensing*, GE-18(3) : 234-240, July 1980.

Madsen and Schhaer-Jacobsen [1978] K. Madsen and H. Schjaer-Jacobsen. Linearly constrained minimax optimization. *Mathematical Programming*, 14 : 208-223, 1978.

McKinnon [1980] G.C. McKinnon. *Contributions to Imaging.* Ph.D thesis, Department of Electrical Engineering, University of Canterbury, Christchurch, New Zealand, 1980.

McKinnon and Bates [1980] G.C. McKinnon and R.H.T. Bates. A limitation on ultrasonic transmission tomography. *Ultrasonic Imaging*, 2(1) : 48-454, January 1980.

Miklin [1970] S.G. Miklin. *Mathematical Physics an Advanced Course*, North Holland, Amsterdam, 1970.

Milne [1980] R.D. Milne. *Applied Functional Analysis.* Pitman, Boston, 1980.

Mitchell and Griffiths [1980] A.R. Mitchell and D.F. Griffiths. *The Finite Difference Method in Partial Differential Equations.* John Wiley, New York, 1980.

Mitchell and Wait [1977] A.R. Mitchell and D.F. Griffiths. *The Finite Element Method in Partial Differential Equations.* John Wiley, New York, 1977.

Mueller *et al.* [1979] R.K. Mueller, M. Kaveh and G. Wade. Reconstructive tomography and applications to ultrasonics. *Proceedings of the IEEE*, 67 : 567-587, 1979.

Müller [1969] C. Müller. *The Mathematical Theory of Electromagnetism.* Springer-Verlag, Berlin, 1969.

Murai and Kagawa [1985] T. Murai and Y. Kagawa. Electrical impedance computed tomography based on a finite element model. *IEEE Transactrions on Biomedical Engineering.* BME-43 : 788-803, 1985.

Murch *et al.* [1988] R.D. Murch, D.G.H. Tan and D.J.N. Wall. Newton-Kantorovich method applied to two-dimensional invers scattering for an exterior Helmholtz problem. *Inverse Problem* 4: 1117-1128, 1988.

Nashed [1971] M.Z. Nashed. The role of differentials in L.B. Rall, editor. *Nonlinear Functional Analysis and its Applications.* Academic Press, New York, 1971.

Newton [1980] R.G. Newton. Inverse scattering. II. Three dimensions. *Journ of Mathematical Physics,* 21(7) : 1698-1715.

Newton [1981] R.G. Newton. Inverse scattering III. Three dimensions, continued. *Journal of Mathematical Physics,* 22(10) : 2191-22(October 1981.

Newton [1982] R.G. Newton. Inverse scattering. IV. Three dimensions : generalized Marchenko construction with bound states, and generalized Gel'fand Levitan equations. *Journal of Mathemati Physics,* 23(4) : 594-604, April 1982.

O'Brien and Wall [1980] D.M. O'Brien and D.J.N. Wall. Radiation from a whip antenna mounted on a sphere. *Journal of Physics D : Applied Physics,* 13 : 2185-2215, 1980.

Oden and Reddy [1976] J.T. Oden and J.N. Reddy. *An Introduction to the Mathematical Theory of Finite Elements,* John Wiley, New Yor 1976.

Oliker [1987] V.I. Oliker. Near radially symmetric solutions of an inverse proble in geometric optics. *Inverse Problems,* 3(4) : 743-756, Novemb 1987.

Parker [1970] R.L. Parker. The inverse problem for electrical conductivity in the mantle. *Geophysical Journal of the Royal Astronomical Society,* 29 : 123-138, 1970.

Parker [1977a] R.L. Parker. Understanding inverse theory. *Annual Review of Earth and Planetary Sciences,* 5 : 35-64, 1977.

Parker [1977b] R.L. Parker. The Fréchet derivative for the one-dimensional electromagnetic induction problem. *Geophysical Journal of the Royal Astronomical Society,* 49 : 543-547, 1977.

Phillips [1973] R.S. Phillips. On the exterior problem for the reduced wave equation. In *Partial Differential Equations, Proceedings of Symposia in Pure Mathematics,* AMS XXIII, 1973.

Polis and Goodson [1976] M.P. Polis and R.E. Goodson. Parameter identification in distributed systems : A synthesizing overview. *Proceedings o the IEEE,* 64 : 45-61, 1976.

Prosser [1969] R.T. Prosser. Formal solutions of inverse scattering problems. *Journal of Mathematical Physics*, 10(10) : 1819-1822, October 1969.

Prosser [1976] R.T. Prosser. Formal solutions of inverse scattering problems II. *Journal of Mathematical Physics*, 17(10) : 1775-1779, October 1976.

Prosser [1980] R.T. Prosser. Formal solutions of inverse scattering problems III. *Journal of Mathematical Physics*, 21(11) : 2648-2653, November 1980.

Rall [1969] L.B. Rall. *Computational solution of nonliner operator equations.* Wiley, New York, 1969.

Ramm [1983] A.G. Ramm. Inverse scattering for geophysical problems. *Physics Letters*, 99A(5) : 258-260, December 1983.

Ramm [1987a] A.G. Ramm. Necessary and sufficient conditions for a function A(θ',θ,k) to be a scattering amplitude corresponding to a reflecting obstacle, *Inverse Problems*, 3(3) : L53-58, August 1987.

Ramm [1987b] A.G. Ramm. Necessary and sufficient conditions on the scatteringf data for the potential to be in L^2 for the Schrödinger operator on the half-line. *Inverse Problems*, 3(4) : L71-L76, November 1987.

Ramm [1987c] A.G. Ramm. Completeness of the products of solutions to PDE and uniqueness theorems in inverse scattering. *Inverse Problems*, 3(4) : L77-L82, November 1987.

Ramm [1988] A.G. Ramm. Multidimensional inverse problems and completeness of the products of solutions to PDE. *Journal of Mathematical Analysis and Applications*, 134 : 211-253, 1988.

Ramm and Waglein [1984] A.G. Ramm and A.B. Waglein. Inverse scattering for geophysical problems. II. Inversion of acoustical data. *Journal of Mathematical Physics*, 25(11) : 3231-3234, November 1984.

Richter [1981a] G.R. Richter. An inverse problem for the steady-state diffusion equation. *SIAM Journal on Applied Mathematics*, 41(2) : 210-221, 1981.

Richter [1981b] G.R. Richter. Numerical identification of a spatially varying diffusivity coefficient. *Mathematics of Computation*, 36 : 375-386, 1981.

Roger [1978] A. Roger. Determination of the index profile of a dielectric plate from scattering data. In P.C. Sabatier, editor. *Applied Inverse Problems*, pp.200-208, Springer-Verlag, Berlin, 1978.

Roger [1981] A. Roger. Newton-Kantorovich algorithm applied to an electromagnetic inverse problem. *IEEE Transactions on antennas and Propagation*, AP29(2) : 232-238, March 1981.

Roger *et al.* [1978] A. Roger, D. Maystre, M. Cadilhac. On a problem of inverse scattering in optics : the dielectric inhomogenous medium. *Journal of Optics*, 9(2) : 83-90, 1978.

Rose *et al.* [1984] J.H. Rose, M. Cheney, and B. DeFacio. The connection between time- and frequency-domain three dimensional inverse scattering techniques. *Journal of Mathematical Physics*, 26(11 2803-2813, November 1985.

Sabatier [1972] P.C. Sabatier. Comparative evolution of inverse problems. (Introduction to an interdisciplinary study of the inverse problems). In L. Colin, editor. *Mathematics of Profile Inversion*, pages 9-2 to 9-20, August 1972. NASA Technical Memorandum X-62, 150. Proceedings of a Workshop held at Ames Research Centre, Moffett Field, California 94035, July 12-16, 1971.

Sabatier [1983] P.C. Sabatier. Theoretical considerations for inverse scattering. *Radio Science*, 18(1) : 1-18, January-February 1983.

Sadeghipour and Yeh [1984] J. Sadeghipour and W.W-G Yeh. Parameter Identification of Groundwater acquifier models : A generalised least squares approach. *Water Resources Research*, 20(7) : 971-979, July 1984.

Schomberg [1978] H. Schomberg. An improved approach to reconstructive ultrasound tomography. *Journal of Physics D : Applied Physic* 11 : L181-L185, 1978.

Schwartz [1967] L. Schwartz. *Cours d'analyse.* Hermann, Paris, 1967.

Sleeman [1982] B.D. Sleeman. The inverse problem of acoustic scattering. *IMA Journal of Applied Mathematics*, 29 : 113-142, 1982.

Sylvester and Uhlmann [1986] J. Sylvester and G. Uhlmann. A uniqueness theorem for an inverse boundary value problem in electrical prospection. *Communications on Pure and Applied Mathemati* 39 : 91-112, 1986.

Sylvester and Uhlmann [1988] J. Sylvester and G. Uhlmann. Inverse boundary value problems at the boundary - continuous dependence. *Communications on Pure and Applied Mathematics*, 41 : 197-21 1988.

Symes [1983a] W. Symes. Some aspects of inverse problems in several-dimension wave propagation. *Proc. Conference on Inverse Problems*, SIAM-AMS Proceedings 14, American Mathematical Society, Providence, RI, 1983.

Symes [1983b] W. Symes. Inverse problems in several-dimensional wave propagation. *International Geophysics and Remote Sensing Digest, IEEE*, 1983.

Symes [1986] W. Symes. Linearization stability for an inverse problem in several dimensional wave propagation. *SIAM Journal on Applied Mathematics*, 17(1) : 132-151, January 1986.

Tan [1988] D.G.H. Tan. *Implementable Multi–Dimensional Inverse Scattering Theory.* Ph.D thesis, Department of Electrical and Electronic Engineering, University of Canterbury, Christchurch, New Zealand, 1988.

Tan and Bates [1988] D.G.H. Tan and R.H.T. Bates. Generalised volume source formulation of diffractioin and a sequence of approximations. *Wave Motion*, 10(5) : 453-462, October 1988.

Tan *et al.* [1988] D.G.H. Tan, R.D. Murch and R.H.T. Bates. Algorithmic implementation of global solution to scalar inverse scattering problem. *Inverse Problems*, 4 : 1129-1146, 1988.

Tijhuis [1981] A.G. Tijhuis. Iterative determination of permittivity and conductivity profiles of a dielectric slab in the time domain. *IEEE Transactions on Antennas and Propagation*, AP-29(2) : 239-295, March 1981.

Tijhuis and Van der Worm [1984] A.G. Tijhuis and C. Van der Worm. Iterative approach to the frequency-domain solution of the inverse-scattering problem for an inhomogenous lossless dielectric slab. *IEEE Transactions on Antennas and Propagation*, AP-32(7) : 711-716, July 1984.

Tikhonov and Arsenin [1977] A.N. Tikhonov and V.Y. Arsenin. *Solutions of Ill–Posed Problems.* V.H. Winston, Washington DC, 1977.

Tracy and Johnson [1983] M.L. Tracy and S.A. Johnson. Inverse scattering solutions by a sinc basis, multiple source, moment method - Part II Numerical evaluation. *Ultrasonic Imaging*, 5(4) : 376-392, October 1983.

Tréves [1975] F. Tréves. *Basic Linear Partial Differential Equations.* Academic Press, New York, 1975.

Tsien and Chen [1978] D.S. Tsien and Y.M. Chen. A pulse-spectrum technique for remote sensing of stratified media. *Radio Science*, 13(5) : 775-783, September-October 1983.

Ursell [1973] F. Ursell. On the exterior problems of acoustics. *Proceedings of the Cambridge Philosophical Society*, 74 : 117-125, 1973.

Vogel [1986] C.R. Vogel. A Banach space ODE framework for inverse scattering via invariant imbedding. *Journal of Mathematical Analysis and its Applications*, 118 : 107-114, 1986.

Wall [1980] D.J.N. Wall. Methods of overcoming numerical instabilities associated with the T-matrix method. In V.K. Varadan and V.V. Varadan, editors. *Acoustic, Electromagnetic and Elastic Wave Scattering – Focus on the T–matrix approach*, pages 269-286, Pergamon Press, New York, 1980.

Wall [1988a] D.J.N. Wall. A uniqueness theorem for the reduced wave equation governing the acoustic wave in a heterogenous medium. *Quarterly Journal of Mechanics and Applied Mathematics*, 41(1) : 141-153, February 1988.

Wall [1988b] D.J.N. Wall. *Uniqueness Theorems for the Inverse Problem of Elastodynamic Boundary Scattering.* Research Report R37-88, Centre for Mathematical Analysis, The Australian National University, Canberra, 1988.

Wall [1988c] D.J.N. Wall. *On the Transmission Problem of Time–Harmonic W[...] Propagation in Heterogenous Media. I. Classical Solutions.* Research Report R41-88, Centre for Mathematical Analysis, The Australian National University, Canberra, 1988.

Wall [1988d] D.J.N. Wall. *On the Transmission Problem of Time–Harmonic Wave Propagation in Heterogenous Media. II. Weak Solutions* Research Report R49-88, Centre for Mathematical Analysis, The Australian National University, Canberra, 1988.

Wall [1989] D.J.N. Wall. On some functional differential equations arising in a time domain inverse scattering problem for a dissipative wave equation. To be submitted to the *Journal of Mathematical Analysis and its Applications.*

Wall *et al.* [1985] D.J.N. Wall, T.S. Yeo and R.H.T. Bates. Inverse scattering and the null field method. In A.J. Devaney and R.H.T. Bates, editor *Inverse Optics II*, pages 25-29, August 1985. Proceedings SPIE volume 558 (the Society of Photo-Optical Instrumentation Engineers).

Weston [1979] V.H. Weston. Nonlinear approach to inverse scattering. *Journal of Mathematical Physics*, 20(1) : 53-59, January 1979.

Weston [1980] V.H. Weston. Inverse problem for the reduced wave equation wit[h] fixed incident field. *Journal of Mathematical Physics*, 21(4) : 758-764, April 1980.

Weston [1984] V.H. Weston. Multifrequency inverse problem for the reduced wave equation with sparse data. *Journal of Mathematical Physics*, 25(5) : 1382-1390, May 1984.

Weston [1985] V.H. Weston. On the convergence of the Rytov approximation fo[r] the reduced wave equation. *Journal of Mathematical Physics*, 26(8) : 1979-1985, August 1985.

Williams [1980] W.E. Williams. *Partial Differential Equations.* Clarendon Press, Oxford, 1980.

Woodhouse [1976] J.H. Woodhouse. On Rayleigh's principle. *Geophysical Journal of the Royal Astronomical Society*, 46 : 11-22, 1976.

Wouk [1979a] A. Wouk. *A Course of Applied Functional Analysis.* Wiley-Interscience, New York, 1979.

Yeh [1986] W.W-G. Yeh. Review of parameter identification procedures in groundwater hydrology : The inverse problem. *Water Resource[s] Research*, 22(2) : 95-108, February 1986.

Yeh and Yoon [1981] W.W-G. Yeh and Y.S. Yoon. Aquifer parameter identification with optimum design in parameterization. *Water Resources Research*, 17(3) : 664-672, June 1981.

APPENDIX

ON AN INVERSE PROBLEM, WITH BOUNDARY MEASUREMENTS, FOR THE STEADY-STATE DIFFUSION EQUATION

Inverse Problems 4 (1988) 995–1012. Printed in the UK

On an inverse problem, with boundary measurements, for the steady state diffusion equation

T J Connolly and David J N Wall†

Department of Mathematics, University of Canterbury, Christchurch, New Zealand

Received 27 October 1987, in final form 27 May 1988

Abstract. The Newton–Kantorovich computational method is applied to the inverse problem of reconstructing a conductivity from given boundary measurements. This paper provides the theoretical analysis necessary to provide rigorous derivations of the Fréchet differential. Linearisations of the non-linear problem are examined and a numerical procedure for reconstructing general conductivities suggested. This procedure is illustrated by reconstructing one-dimensional conductivities.

1. Introduction

The classical direct problem associated with the partial differential equation

$$\nabla \cdot [f(x)\nabla u(x)] = 0 \qquad x \in R^n \qquad n = 2 \text{ or } 3 \tag{1.1}$$

is to determine u, given f and appropriate boundary conditions on the boundary $\partial\Omega$ of the bounded, simply connected open region Ω. We shall assume the boundary $\partial\Omega$ is a C^1 mapping of a compact interval $I \subset R$ into R^n. The boundary conditions we shall consider are either Dirichlet

$$u(x) = g(x) \qquad x \in \partial\Omega \tag{1.2}$$

or the normalised Neumann boundary condition

$$f(x)\frac{\partial u}{\partial v} = g(x) \qquad x \in \partial\Omega \tag{1.3}$$

where $\partial/\partial v$ denotes the directional derivative in the direction of the unit outward normal vector $\hat{v}$ to $\partial\Omega$.

The inverse or identification problem we shall examine in this paper is to determine the spatially varying function f from knowledge of $u(x)$ for $x \in \partial\Omega$; that is certain measurements of u on the boundary. These measurements consist of the following.

(i) If Dirichlet conditions are specified on $\partial\Omega$ then $f\,\partial u/\partial v$ is measured on $\partial\Omega$.

(ii) If Neumann conditions are specified on $\partial\Omega$ then u is measured on $\partial\Omega$.

Of course these are not the only permissible measurements, but a necessary condition for this problem is that the measurement set must be independent of the specified set.

† Visiting: Centre for Mathematical Analysis, Australian National University, Canberra, ACT 2601, Australia.

0266–5611/88/040995 + 18 $02.50

The inverse problem for equation (1.1) is of considerable importance as it arises from several physical problems. A major application is in electrical conductivity imaging, or 'impedance tomography' as the medical technique of non-invasive conductivity measurement is called (see [1–3]). It also arises in two geophysical problems. The first is in geophysical prospecting by electrical probing, where again f represents a conductivity (see [4]). The second has applications in the study of groundwater flow and oil reservoirs; this problem is, however, not generally of the boundary measurement type (see [5, 6]).

In this paper we assume that the measurements are known to arise as a response to a particular f^*. If this is not the case then the validity of the model equation (1.1) will be in doubt. However, the measurements may be contaminated by noise and so computational methods of solution that are not invalidated by this assumption are examined. It can be profitable, however, to examine the characterisation problem that is associated with the inverse problem. The characterisation problem can be stated as follows. Given some measurements, find if they arise from an f in equation (1.1). Mathematically this means that the measurements must lie in the correct function space, or subspace. As an example of this, if f, $\partial\Omega \in C^\omega$ then the measurements must also be in C^ω or perhaps a subset of C^ω. The characterisation problem has been recently examined in a related problem [7].

The next difficulty which must be examined is the question of the uniqueness from a given set of measurements. To solve the inverse problem the boundary conditions are varied so giving additional information with which to reconstruct f^*. The question as to which boundary conditions can be specified so that the resulting measurements uniquely determine an arbitrary conductivity is an open one at the present time. However, this question is obviously of considerable theoretical and practical importance.

Kohn and Vogelius in a series of papers [8–10] have gone some way towards answering this central uniqueness question with the following result.

If the open region Ω has a boundary $\partial\Omega \in C^\infty$ and f^* is a positive piecewise real analytic function, then it is uniquely determined by knowledge of $f\,\partial u/\partial\upsilon$ on $\partial\Omega$ for all possible Dirichlet data $g \in H^{1/2}(\partial\Omega)$.

Here the Sobolev space $H^{1/2}$ is defined in §2. We point out that this result includes practically all f^* of computational interest and even handles f^* having edges. This is because it is the 'weak' formulation of (1.1) that is of concern here and so with the given assumptions, the solution to the direct problem is such that u is at least in $H^1(\Omega)$. We conjecture that Kohn and Vogelius's result also applies if measurements (ii) instead of (i) are used. To our knowledge no proof of this conjecture exists, but a small change to their argument would include this case. Other authors have considered the uniqueness of related identification problems but these are not of so much interest to us here, as they require $f \in C^\infty(\Omega)$ [11, 12].

In any computational solution of the inverse problem the knowledge that the mapping from f to the measurements is continuous is important. We consider the application of the Newton–Kantorovich method to the aforementioned non-linear inverse problem. The Newton–Kantorovich method proceeds by local linearisation, so of immediate concern with such methods is the justification for differentiability. We provide a rigorous proof of differentiability and continuity of an important operator for this problem, thereby providing the theoretical analysis necessary to justify many of the computational schemes which have been developed for this problem [13–15]. The reason why we have chosen the Newton–Kantorovich method is that it is a very general approach having applications to many inverse problems differing substantially from (1.1). The application of the Newton–Kantorovich method for the solution of inverse problems in general has been investigated in [16], see also applications in [17–19]. Provided the non-linear operator admits a linearisation this method offers the following desirable additional features.

(i) Quadratic convergence in the vicinity of a local solution.

(ii) The method can be made to have global convergence by incorporating line searches.

(iii) The functional in the method can easily be modified to include stabilising features.

In §2 we introduce the inverse problem and discuss its non-linear and ill-conditioned nature. We also define the Newton–Kantorovich method as applied to this problem. Section 3 contains our central results on the linearisation of the non-linear operator. It also contains a result ensuring a solution even if the measurements are marred by noise. In §4 we consider an important approximation to the non-linear operator, namely a particular linear approximation. It is also shown that this linear approximation has a unique solution and leads to a set of uncoupled one-dimensional moment equations. Section 5 completes this paper by providing numerical results of our methods on a simple example.

2. Derivation of an iterative scheme for solution of the identification problem

In the following we consider only specified Neumann boundary conditions on the direct problem (1.1) and where measurements are made of the resulting field on $\partial\Omega$. We consider only the Neumann boundary condition for simplicity; the Dirichlet boundary condition follows our work in a similar manner.

The field $u(x)$ is a functional of the unknown function f and the boundary data g. To make this more explicit we shall often write the field as $u(f;\, g;\, x)$. The direct problem is then governed by the equations

$$\begin{aligned} &\nabla\cdot[f(x)\nabla u(f;g;x)]=0 && x\in\Omega \\ &f(x)\frac{\partial}{\partial v}u(f;g;x)=g(x) && x\in\partial\Omega. \end{aligned} \tag{2.1}$$

The classical solution of (2.1) is such that $u\in C^2(\Omega)\cap C^1(\partial\Omega)$ and $f\in C^1(\Omega)\cap C(\partial\Omega)$. The direct problem as it stands does not have a unique solution as constant functions are in the null space of this operator equation. To ensure the existence of a solution, the data must lie in the range of the operator, hence we have the solvability condition

$$\int_{\partial\Omega} g(x)\,\mathrm{d}S=0. \tag{2.2}$$

Then to produce a unique solution, $u(f;g;x_0)$ is specified for some $x_0\in\Omega$. The energy of the solution of (2.1) is important in the following and is given by

$$E_f(g)=\int_\Omega f|\nabla u|^2\,\mathrm{d}x. \tag{2.3}$$

To prove Fréchet differentiability in §3, we shall have to consider f and u being members of appropriate Banach spaces. For the inverse problem we require as little restriction on f as possible, so we choose $f \in F$ where $F = \{f \in L^\infty(\Omega)\colon \inf_\Omega f > 0\}$. The weak formulation of (2.1) is then the most appropriate, and is

$$\int_\Omega f \nabla u \cdot \nabla w \, \mathrm{d}x - \int_{\partial\Omega} f w g \, \mathrm{d}S = 0 \qquad \text{for all } w \in H^1(\Omega). \tag{2.4}$$

A solution of the direct problem (2.1) is said to be a weak solution if it is a solution of (2.4). Obviously a classical solution of (2.1) is also a solution of (2.4), but not necessarily the other way around. The weak solution u is then such that $u \in H^1(\Omega)$.

We shall now provide a definition of the Sobolev spaces used throughout this paper (see [20]). Prior to this we introduce some standard distribution notation. We define $\mathfrak{D}$ as the space of test functions $\varphi \in C_0^\infty(R^n)$ with the space $\mathfrak{D}'$ denoting its dual. The elements of $\mathfrak{D}$ are called distributions or generalised functions. We define, on the functions on R^n, the semi-norms q_{jk} where

$$q_{jk}(u) = \sup_{x \in R^n} \{(1 + |x|^2)^{j/2} |D^\alpha u(x)|;\, |\alpha| < k\} \qquad \text{for all } j, k \in \mathbb{Z}_+.$$

Then the space $\mathcal{S}(R^n)$ consists of the functions u of rapid decay on R^n for which each q_{jk} is finite, with a Fréchet space topology determined by these semi-norms. Its dual is denoted by $\mathcal{S}'(R^n)$ and is called the space of tempered distributions. We denote by $H^s(\boldsymbol{R}^n)$ the space of generalised functions $u \in \mathcal{S}'$ whose Fourier transform is square-integrable in $\boldsymbol{R}^n$ for the measure $(1 + |\xi|^2)^s$, where $\xi \in \boldsymbol{R}^n$ is the Fourier transform variable and $s \in \boldsymbol{R}$. This norm is denoted by $\| \cdot \|_s$. By defining $\mathfrak{D}_\Omega$ as the totality of test functions from $\mathfrak{D}$ having their support in Ω, it then follows that $H^s(\Omega)$ can be defined as the totality of those generalised functions from $\mathfrak{D}'_\Omega$, that are the restrictions to Ω of those generalised functions belonging to $H^s(R^n)$. In $H^s(\Omega)$ we introduce the norm

$$\|u\|_{s,\Omega} = \inf \|u^c\|_s$$

where the infimum is taken over all those generalised functions $u^c \in H^s(\boldsymbol{R}^n)$ whose restrictions to Ω coincide with u.

If $\Omega \in \boldsymbol{R}^n$ is an open subset, then we denote by $H^s_{\mathrm{loc}}(\Omega)$ the space of distributions $u \in \mathfrak{D}'$ such that $\varphi u \in H^s$ for all $\varphi \in C_0^\infty(\Omega)$. $H^s_{\mathrm{loc}}(\Omega)$ is equipped with the family of semi-norms $\|\varphi u\|_s$. If we have a smooth compact manifold X then $H^s_{\mathrm{loc}}(X) = H^s(X)$ and the dual $(H^s(X))' = H^{-s}(X)$ We use these semi-norms on $H^s(\partial\Omega)$ where $\partial\Omega$ is a compact $\boldsymbol{R}^{n-1}$ manifold.

When the $L_\infty(\Omega)$ norm is used, we denote it by $\|\cdot\|_{\infty,\Omega}$. The specified data g will be considered to be in $H^{-1/2}(\partial\Omega)$ and we note that the exact measurements are in the smoother space $H^{1/2}$.

If f has corners or edges, then when considering classical solutions of (2.1) it is necessary to impose an edge condition on the solution to ensure uniqueness. An edge condition that will give sufficiency conditions for a unique solution is that the energy density—defined by the integrand of the right-hand side of (2.3)—is integrable over any sub-region of Ω, even if this sub-region contains singularities of the field. The edge condition will therefore be automatically satisfied by any weak solution of (2.1), as then $u \in H^1(\Omega)$. This is another reason for considering weak solutions because in an inverse problem there is no *a priori* knowledge as to whether or not f possesses edges.

The choice $f \in F$ means that the equation (2.1) will not possess a classical solution throughout Ω. However a solution of the weak formulation (2.4) will automatically satisfy the classical jump conditions required across a surface, denoted by Γ, across which f has a discontinuity. If $\hat{v}$ is a unit normal vector on a surface Γ, the difference between the values taken by the field φ on the side of Γ towards which and away from which $\hat{v}$ is directed, is defined as the jump of φ on Γ and is denoted by $[\![\varphi]\!]_\Gamma$. Then one of the classical jump conditions is

$$\left[\!\!\left[f\frac{\partial u}{\partial v} \right]\!\!\right]_\Gamma = 0. \tag{2.5}$$

The other classical jump condition required across such a surface is $[\![u]\!]_\Gamma = 0$, that is $u \in C(\Omega)$. This will be achieved by the weak solution if $u \in H^2(\Omega)$—by the Sobolev embedding theorem—when $n = 2$ or 3. This increased regularity of the weak solution is achieved provided Ω satisfies certain smoothness properties (see [21]).

It is convenient to sometimes attach a subscript to the specified data g_p for the problem (2.1), the associated solution then being denoted by u_p. When (2.1) is to hold for u_q, and it is multiplied by u_p we can show by application of the divergence theorem applied to the result that

$$\int_\Omega f \nabla u_q \cdot \nabla u_p \, \mathrm{d}x = \int_{\partial\Omega} u_p f \frac{\partial u_q}{\partial v} \, \mathrm{d}S \tag{2.6}$$

where the right-hand side represents the dual pairing $H^{1/2}(\partial\Omega) \otimes H^{-1/2}(\partial\Omega)$. When $p = q$ the left-hand side represents the energy of the solution (see (2.3)). Then in particular if $f\partial u_p/\partial v = g_p$ and $p = q$ the right-hand side is considered also as a measure of the energy in Ω; $f\partial u/\partial v$ being the weakly defined flux.

If the measurements of u on $\partial\Omega$ are denoted by U, perhaps the most obvious formulation of the inverse problem is the non-linear operator equation

$$R(f) \equiv u(f; g_q; x) - U(g_q; x) = 0 \qquad x \in \partial\Omega. \tag{2.7}$$

It is important to note that (2.7) is not the only non-linear operator available for this problem. Indeed any continuous linear functional of the right-hand side is also suitable.

Clearly, if f satisfies the conditions required in (2.1) and the measurements are exact, then the existence of a solution to (2.7) is assured by lemma 1 in §3. By considering R as an affine operator mapping u in Ω onto its boundary values on $\partial\Omega$, we see that it is a trace operator [22, p249], hence $u \in H^{1/2}(\partial\Omega)$. It follows when considering exact measurements and weak solutions $U \in H^{1/2}(\partial\Omega)$. R can be considered as $R{:}F(\Omega) \mapsto H^{1/2}(\partial\Omega)$. It should be noted that this map will not be surjective.

To clarify this point we will illustrate that R will often be a completely continuous (that is, compact and continuous) operator, thereby implying it will have an unbounded inverse.

Consider a case in which f is regular in the neighbourhood of $\partial\Omega$. We will assume f is at least C^1 in this neighbourhood. Then a local regularity result (see [21, ch 8]) implies that u is at least in H^2 in this neighbourhood. This together with the assumption that $\partial\Omega$ is a C^2 boundary means that the trace of u will be at least in $H^{3/2}(\partial\Omega)$, which by Rellich's embedding theorem is compactly embedded in $H^{1/2}(\partial\Omega)$. The composition result for a bounded continuous and a completely continuous operator can then be used on $R{:}F(\Omega) \mapsto H^{1/2}(\partial\Omega)$ to imply this map is completely continuous and hence that R^{-1} if it exists will be unbounded. The identification problem will therefore be ill-posed in the sense of Hadamard, as the solution will not depend continuously upon the data U. The consequent regularisation which must be carried out will be discussed further in §3.

To solve (2.7) for f, $R(f)$ is linearised and a series of linear subproblems is solved; this leads to the Newton–Kantorovich iterative scheme:

$$f^{(k+1)} = P(f^{(k)} + s^{(k)}) \qquad k = 0, 1, 2, \ldots \tag{2.8}$$

given a positive $f^{(0)}$ and where P is a projection operator ensuring that $f^{(k+1)} > 0$. In (2.8) the update $s^{(k)}$ is the solution of the linear operator equation.

$$R'(f^{(k)})s^{(k)} = -R(f^{(k)}). \tag{2.9}$$

To utilise this method the Fréchet derivative of $R(f)$ with respect to f, denoted by R', must be known. We shall not consider the operator R' any further here as it will involve the calculation of Green functions and this produces a method with excessive computational requirements; but see [16]. So we will now look at a method which only requires computation of the direct problem solutions.

Define the operator

$$Q(f) = \int_{\partial\Omega} g_p(x)[u(f; g_q; x) - U(g_q; x)]\mathrm{d}S \qquad g_p, g_q \in H^{-1/2}(\partial\Omega) \tag{2.10}$$

where this definition comes from the inner product of $R(f)$ with the functions g_p. Here the g_p, g_q are specified boundary functions on $\partial\Omega$, and to obtain reconstructions of f the g_p, g_q are taken from a basis in $H^{-1/2}(\partial\Omega)$. When $p = q$ in (2.10) the energy of the direct problem solution (see equation (2.6) and what follows) is required to match that of the measurements. However we will show in §4, by example, that $p \neq q$ is required to obtain reconstructions when the boundary data are taken from such a basis.

The identification problem can now be stated as the non-linear functional equation

$$Q(f) = 0 \tag{2.11}$$

where $Q: F(\Omega) \mapsto R$. In fact Q can be considered as a non-linear generalised moment equation. Similar to (2.7) if f satisfies the conditions required in (2.1) and the measurements are exact, then the existence of a solution to (2.11) is assured. To solve (2.11) for f, $Q(f)$ is linearised with the Newton–Kantorovich iterative scheme (2.8), where now the update $s^{(k)}$ is the solution of the linear operator equation

$$Q'(f^{(k)})s^{(k)} = -Q(f^{(k)}). \tag{2.12}$$

To utilise this method the Fréchet derivative Q' is required, the differential is

$$Q'(f)s = -\int_{\Omega} \nabla u(f; g_p; x) \cdot \nabla u(f; g_q; x) s(x)\, \mathrm{d}x. \tag{2.13}$$

Derivation of this differential is given in the proof of theorem 1 in §3. We note that (2.12) is a linear moment problem for the update function $s^{(k)}(x)$, where $x \in \Omega \subset R^n$.

Later we shall need the fact that the functional equation (2.13) is a symmetric functional of g_p and g_q, provided U represents exact measurement data. This follows immediately from the observation

$$\int_{\partial\Omega} g_p(x)u(f; g_q; x)\, \mathrm{d}S = \int_{\partial\Omega} g_q(x)u(f; g_p; x)\, \mathrm{d}S \tag{2.14}$$

which is deduced from equation (2.6).

3. Fréchet differentiability and considerations of well posedness

Before proceeding with any computational implementation of the method advocated for the non-linear moment operator $Q(f)$ derived in the last section, we must examine the existence of the Fréchet derivative for Q defined on suitable function spaces. Prior to proving differentiability we need the results of three lemmas. These show respectively

(i) continuous dependence of the solution of the Neumann direct problem on the boundary data g;

(ii) continuous dependence of ∇u on the function f;

(iii) $Q'(f)$ is a bounded operator.

In this section functional dependence upon the independent variable x will be omitted for brevity where convenient.

Lemma 1. If $f \in F(\Omega)$, and $g \in H^{-1/2}(\partial\Omega)$, then there exists a solution $u \in \overset{\circ}{H}{}^1(\Omega)$ of (2.1), where $\overset{\circ}{H}{}^1(\Omega)$ is the quotient space of $H^1(\Omega)$ modulo the constant functions, and also u satisfies the well posedness condition

$$\|u\|_{1,\Omega} \leqslant C(f, \Omega)\|g\|_{-1/2,\partial\Omega}. \tag{3.1}$$

Proof. Follows standard weak theory for partial differential equations—see [22].

Lemma 2. If $\nabla\cdot(f_1\nabla u_1)=0$ and $\nabla\cdot(f_2\nabla u_2)=0$, both for $x \in \Omega$ then

(i)

$$\int_\Omega \nabla u_1\cdot\nabla u_2(f_1-f_2)\,\mathrm{d}x = \int_{\partial\Omega}\left(f_1 u_2\frac{\partial u_1}{\partial \upsilon} - f_2 u_1 \frac{\partial u_2}{\partial \upsilon}\right)\mathrm{d}S.$$

(ii) If also

$$f_1\frac{\partial u_1}{\partial \upsilon} = f_2\frac{\partial u_2}{\partial \upsilon} \qquad x \in \partial\Omega$$

then

$$\frac{\|\nabla(u_1-u_2)\|_{0,\Omega}}{\|\nabla u_1\|_{0,\Omega}} \leqslant \frac{\|f_1-f_2\|_{\infty,\Omega}}{\inf_\Omega f_2}.$$

Proof. (i) From initial assumptions

$$\int_\Omega u_1\nabla\cdot(f_2\nabla u_2)\,\mathrm{d}x = 0$$

then utilising, from the appendix, equation (A1)

$$\int_\Omega f_2\nabla u_1\cdot\nabla u_2\,\mathrm{d}x = \int_{\partial\Omega} f_2 u_1\frac{\partial u_2}{\partial \upsilon}\,\mathrm{d}S. \tag{3.2}$$

Similarly one can show

$$\int_\Omega f_1\nabla u_1\cdot\nabla u_2\,\mathrm{d}x = \int_{\partial\Omega} f_1 u_2\frac{\partial u_1}{\partial \upsilon}\,\mathrm{d}S. \tag{3.3}$$

By subtracting (3.2) from (3.3) we get the required result.

(ii) From the initial assumptions

$$\nabla\cdot[(f_1-f_2)\nabla u_1]=\nabla\cdot[f_2\nabla(u_2-u_1)]$$

and so

$$\int_\Omega (u_1-u_2)\nabla\cdot[(f_1-f_2)\nabla u_1]\,\mathrm{d}\boldsymbol{x}=\int_\Omega (u_1-u_2)\nabla\cdot[f_2\nabla(u_2-u_1)]\,\mathrm{d}\boldsymbol{x}. \tag{3.4}$$

Applications of (A1) to both sides of (3.4) and utilising assumptions for part (ii) shows

$$\int_\Omega (f_1-f_2)\nabla u_1\cdot\nabla(u_1-u_2)\,\mathrm{d}\boldsymbol{x}=\int_\Omega f_2|\nabla(u_1-u_2)|^2\,\mathrm{d}\boldsymbol{x}. \tag{3.5}$$

The Cauchy–Schwarz inequality applied to the left-hand side of (3.5) and use of equation (3.5) now gives

$$\|(f_1-f_2)\nabla u_1\|_{0,\Omega}\geqslant\inf_\Omega f_2\,\|\nabla(u_1-u_2)\|_{0,\Omega}$$

so that

$$\|f_1-f_2\|_{\infty,\Omega}\|\nabla u_1\|_{0,\Omega}\geqslant\inf_\Omega f_2\,\|\nabla(u_1-u_2)\|_{0,\Omega}$$

as required. The result (ii) follows Richter [5]; we have included this proof for completeness.

Lemma 3. The mapping $Q'(f)$: $F(\Omega)\mapsto \boldsymbol{R}$ is a continuous linear functional.

Proof. From (2.13)

$$Q'(f)s=-\int_\Omega \nabla u(f;g_p)\cdot\nabla u(f;g_q)s\,\mathrm{d}\boldsymbol{x}$$

and so

$$|Q'(f)s|\leqslant\int_\Omega \nabla u(f;g_p)\cdot\nabla u(f;g_q)|\mathrm{d}\boldsymbol{x}\|s\|_{\infty,\Omega}$$

and by the Cauchy–Schwarz inequality

$$|Q'(f)s|\leqslant\|\nabla u(f;g_p)\|_{0,\Omega}\|\nabla u(f;g_q)\|_{0,\Omega}\|s\|_{\infty,\Omega}.$$

From lemma 1 it follows that $\|\nabla u(f;\ g)\|_{0,\Omega}\leqslant C\|g\|_{-1/2,\partial\Omega}$ for any boundary data $g\in H^{-1/2}(\partial\Omega)$ then

$$|Q'(f)s|\leqslant C(f,\Omega,g_p,g_q)\|s\|_{\infty,\Omega}.$$

It follows that Q' is a bounded linear operator, and hence continuous. Its norm—an operator norm—is bounded by the infimum of C for fixed g_p, g_q, that is

$$\|Q'(f)\|=\inf C(f,\Omega,g_p,g_q). \tag{3.6}$$

A norm which will be independent of the particular base set $\{g_p\}$ can be found by finding the infimum of C to be also over the $\{g_p\}$, while restricting the norm such that

$\|g_p\|_{-1/2,\partial\Omega}=\|g_q\|_{-1/2,\partial\Omega}=1$. We shall use this latter norm on the operator Q and its derivatives in the following.

It follows from lemma 2(ii) that ∇u depends continuously on f. We can now state the differentiability result.

Theorem 1. If Ω is a bounded domain with a C^1 boundary and with Neumann boundary conditions such that g_p, $g_q \in H^{-1/2}(\partial\Omega)$ then the non-linear functional $Q:F\mapsto \boldsymbol{R}$ given by (2.10) is Fréchet differentiable with Fréchet differential given by (2.13).

Proof. Define

$$\begin{aligned} w(f;s) &= Q(f+s)-Q(f)-Q'(f)s \\ &= \int_{\partial\Omega} g_p[u(f+s;g_q)-U(g_q)]\,\mathrm{d}S \\ &\quad -\int_{\partial\Omega} g_p[u(f;g_q)-U(g_q)\,\mathrm{d}S+\int_{\Omega}\nabla u(f;g_p)\cdot\nabla u(f;g_q)s\,\mathrm{d}\boldsymbol{x}. \end{aligned} \tag{3.7}$$

Now first just consider the first two integrals on the right-hand side of (3.7). If the symmetry property (2.14), together with the boundary conditions satisfied by the solutions $u(f+s;\, g_q)$ and $u(f;\, g_q)$ are combined with lemma 1(i) the two integrals become

$$\int_{\partial\Omega}[g_q u(f+s;g_p)-g_p u(f;g_q)]\,\mathrm{d}S=-\int_{\Omega}\nabla u(f+s;g_p)\cdot\nabla u(f,g_q)s\,\mathrm{d}\boldsymbol{x}.$$

Then it follows (3.7) can be written

$$w(f;s)=-\int_{\Omega}\nabla u(f,g_q)\cdot\nabla[u(f+s;g_p)-u(f,g_p)]s\,\mathrm{d}\boldsymbol{x}$$

and

$$|w(f;s)|\leqslant\int_{\Omega}|\nabla u(f,g_q)\cdot\nabla(u(f+s;g_p)-u(f,g_p))|\,\mathrm{d}\boldsymbol{x}\|s\|_{\infty,\Omega}.$$

By using the Cauchy–Schwarz inequality on this equation we get

$$|w(f;s)|\leqslant\|\nabla u(f,g_q)\|_{0,\Omega}\|\nabla[u(f+s;g_p)-u(f,g_p)]\|_{0,\Omega}\|s\|_{\infty,\Omega}.$$

Lemma 1(ii) applied to the second norm on the right-hand side of this inequality then shows

$$\|\nabla[u(f+s;g_p)-u(f;g_p)]\|_{0,\Omega}\leq\|s\|_{\infty,\Omega}\|\nabla u(f+s;g_p)\|_{0,\Omega}/\inf_{\Omega} f.$$

The last two inequalities show the quantity

$$\frac{|w(f;s)|}{\|s\|_{\infty,\Omega}}\leq\|\nabla u(f,g_q)\|_{0,\Omega}\|\nabla u(f+s;g_p)\|_{0,\Omega}\|s\|_{\infty,\Omega}/\inf_{\Omega} f$$

and in the limit as $\|s\|_\infty\to 0$ we have

$$\lim_{\|s\|_{\infty,\Omega}\to 0}\frac{\|w(f;s)\|}{\|s\|_{\infty,\Omega}}=0 \tag{3.8}$$

where use is made of lemma 1 and the norm on w is defined as discussed following (3.6). Equation (3.8) together with lemma 3 gives the required result.

It follows directly from theorem 1 that the operator Q is continuous with respect to f.

In the presence of measurement noise we generally have

$$U(g;x)\neq u(f^*;g;x) \qquad x\in\partial\Omega$$

and so a solution of our operator equations may not exist. In order to guarantee the existence of a solution we use *a priori* information on its smoothness to reformulate the inverse problem as a minimisation over a compact set (see [23]). This constitutes the Tikhonov selection technique for numerical regularisation.

When g_p, g_q are chosen from a basis set in $H^{-1/2}(\partial\Omega)$ with unit norm, we can write the operator Q as $Q(f;g_p;g_q)$ and could consider the norm for fixed f,

$$\|Q(f)\|=\sup_{g_p,g_q\in G}|Q(f;g_p;g_q)| \tag{3.9}$$

where $G=\{g\in H^{-1/2}(\partial\Omega)\colon \|g\|=1\}$. Then we can pose the minimisation problem

$$\min_{f\in F_0}\|Q(f)\|^2 \tag{3.10}$$

where F_0 is a compact subset of F. A norm more computationally convenient than (3.9) can be found by restricting the boundary data to a N-dimensional subset of $H^0(\partial\Omega)$. Then we pose the minimisation problem as (3.10), but with the norm now being the Frobenius norm

$$\|Q(f)\|=\left\{\sum_{p,q}^{N}|Q(f;g_p;g_q|^2\right\}^{1/2}. \tag{3.11}$$

However, it is convenient instead to think of (3.11) as a vector 2-norm. This is done by considering $Q_r(f)=Q(f;g_p;g_q)$, where there is a bijective mapping from the subscripts $p,q\to r$; therefore $1\leq r\leq N\times N$. We could then add subscript 2 to the norm symbol on the left-hand side of (3.11). With the problem now set as a minimisation the following result can be obtained.

Theorem 2. There exists a solution of the minimisation problem (3.10) with norm (3.11), provided F_0 is compact and the conditions of theorem 1 hold.

Proof. From theorem 1, $Q(f)$ is Fréchet differentiable and so is a continuous operator. The norm in (3.11) is continuous: hence the result follows from the compactness of F_0.

One possible choice for F_0 suitable for computational purposes is

$$F_0 = \{f \in H^m(\Omega): \|f\| \leqslant M, f \geqslant c > 0\}.$$

The constants M and c are given *a priori* and the compactness of F_0 follows from the compactness of the embedding $H^m(\Omega) \to L^\infty(\Omega)$ (see Adams [24, ch 5]). This would require $m = 2$ if f is two or three dimensional. If this choice of F_0 were to be used the resulting reconstructions of a discontinuous f would be smoothed. However, if discontinuous reconstructions are desired the solution set F_0 could be chosen a finite-dimensional subspace of $L^\infty(\Omega)$, such as the splines of degree zero; if we add the requirement $\|f\|_\infty \leqslant M$, then this F_0 also has the required compactness property. We shall use such a solution set in §5. This Tikhonov selection regularisation scheme has been used in solving inverse wave scattering problems [25]. The regularisation parameter M restricts the compact space in which the solution is to be found, and this parameter is varied until convergence is manifest.

Even when we have assured ourselves that the minimisation problem (3.10) has a solution, say $\hat{f}$, it may not be close to the f^*. What one also requires is that

$$\|\hat{f} - f^*\|_{\infty,\Omega} \leqslant \gamma \|u(f^*; g; x) - U(g; x)\| \qquad x \in \partial\Omega$$

and γ is known. The inverse problem will be well understood when such inequalities are found for it. Some results of this kind are available for other inverse problems [26, ch 8, 27, 28].

It should be noted that computationally the problem is not solved as a full minimisation problem which would require estimations of second derivatives. Instead (3.10) is used to solve (2.11) with the Gauss–Newton method. With this approach (2.12) together with (2.8) is used, but the update equation (2.12) is solved by a least-squares approach. This enables the number of measurements to be overdetermined; a desirable feature with measurement noise. A line search is usually incorporated to determine the magnitude of $s^{(k)}$ (see, e.g., [29]). With this approach the Fréchet differential of Q is again important and is what is required.

4. The linearised problem

In the non-linear problem (2.11) if an approximation denoted by f^0 is known to the solution f^*, then

$$\|Q(f^*) - [Q(f^0) + Q'(f^0)s]\| = o[\|f^* - f^0\|) \tag{4.1}$$

as $f^0 \to f^*$, and where $s = f - f^0$. Fréchet differentiability of Q, as shown in theorem 1, ensures (4.1) is valid. Equation (4.1) implies the linearisation of Q, namely the term in square brackets inside the norm symbol on the right-hand side of equation (4.1), is a *good* approximation to Q near f^* if $\|f^* - f^0\|_{\infty,\Omega}$ is *small enough*. The solution of the linearised inverse problem

$$Q'(f^0)s = -Q(f^0) \tag{4.2}$$

namely $f^{(1)}=s+f^{0}$, may then be expected to provide a good approximation to f^*, and some numerical results we present in §5 confirm this.

Other authors have considered the linear versions of several inverse problems involving the wave equation [30, 31]. They use the well known Born approximation to linearise their problems.

Calderon [32] has shown that there is a unique solution to the inverse problem which is linearised about an f constant over Ω given knowledge of the energy E_f from all possible Dirichlet boundary conditions. He did this by showing that the Fréchet differential of the map from f to E_f is injective, for f a constant. In this paper he also gives a method for approximating f, when f is close to constant.

We are interested here however, in the practical situation of reconstruction of non-smooth f where independent boundary data are chosen from an N-dimensional subspace of $H^0(\partial\Omega)$. When $n=2$, use of the energy will only enable a one-dimensional projection of the two-dimensional f to be constructed. We shall show in the following that, for the case when $n=2$ and Ω is a circular domain, knowledge of the energy can only be used to reconstruct radially symmetric f. But by utilising the quantities given by the right-hand side of (2.6), when p is not always equal to q, we shall show that a two-dimensional f can be reconstructed. It should be noted when using the known value of the energy it corresponds to using *only* the quantities when $p=q$. We shall also show that there is a unique solution to this inverse problem linearised about an f constant over Ω. This shows that our approach produces at least a *locally* unique solution to the non-linear problem. Our method leads to a set of uncoupled one-dimensional moment problems which can be solved with computational efficiency.

We now discuss the computational method of solving the linearised problem (4.2) for a particular problem geometry, when $n=2$. Take Ω to be the open region bounded by a circle centred on the origin and of radius unity. This in fact involves no loss in generality, as by a partition of unity, any other open simply connected two-dimensional region can be mapped into this circle. We set up a circular polar coordinate system (r, θ) at the origin. As the specified data are to be independent, and to come from a $(2N+1)$-dimensional subspace of $H^{-1/2}(\partial\Omega)$ it is computationally convenient to take them from the trigonometric polynomial set, namely

$$\left\{ \begin{matrix}\cos\\ \sin\end{matrix} (p\theta) \right\}_{p=0}^{N}$$

note $H^0 \subset H^{-1/2}$. When f in (2.1) is not spatially varying, and given by f^0, the solution of (2.1) is

$$u_p^{\substack{e\\o}} = r^p \begin{matrix}\cos\\ \sin\end{matrix} (p\theta)/f^0 + \text{constant} \tag{4.3}$$

where the superscripts e, o attached to u are taken to mean that the even and odd trigonometric polynomials are respectively to be used on the right-hand side of (4.3). The even or odd trigonometric polynomials are to be used in the solution $u_p^{\substack{e\\o}}$ depending upon whether the boundary data g_p are of the even or odd type.

We then resolve the difference between the field $u_p(f; x)$ and the measured field $U_p(x)$ on $\partial\Omega$ into the Fourier amplitudes $A_{p,m}(f^*, f)$ and $B_{p,m}(f^*, f)$, so that

$$u_p(f; x) - U_p(x) = \sum_{m=0}^{\infty} \varepsilon_m [A_{p,m} \cos(m\theta) + B_{p,m} \sin(m\theta)] \qquad x \in \partial\Omega \tag{4.4}$$

where ε_m is the Neumann factor. We note $B_{p,0}=0$ throughout the following, and we have dropped the arguments f^*, f from the terms $A_{p,m}$, $B_{p,m}$. Use of (4.3), (4.4) and (2.13) in (4.2) then shows

$$\int_0^{2\pi}\int_0^1 r^{p+q-1} \begin{matrix}\cos\\ \sin\end{matrix}[(p-q)\theta]s(r,\theta)\,\mathrm{d}r\,\mathrm{d}\theta = 2\pi(f^0)^2 \begin{matrix}+A_{p,q}(f)\\ -B_{p,q}(f)\end{matrix} \qquad 0\leqslant p, q<\infty. \tag{4.5}$$

We note that only the equations $p\geqslant q$ are necessary in (4.5) because of (2.14). To solve this linear system of moment equations set

$$s^{(0)}(r,\theta)=\sum_{m=0}^{N}\varepsilon_m[a_m(r)\cos(m\theta)+b_m(r)\sin(m\theta)] \qquad 0\leqslant r\leqslant 1, 0\leqslant\theta\leqslant 2\pi$$

and substitute this in (4.5), to give the dual uncoupled one-dimensional moment system

$$\int_0^1 r^{n+2q-1}\begin{matrix}a_n(r)\\ b_n(r)\end{matrix}\,\mathrm{d}r=(f^0)^2\begin{matrix}A_{n+q,q}\\ -B_{n+q,q}\end{matrix} \qquad 0\leqslant n, q\leqslant N \tag{4.6}$$

where we have set $n=p-q$. It is now clear that, for the linearised problem (4.2), the leading diagonal of the matrix $A_{p,q}$ is used to reconstruct the radial part $a_0(r)$ of $s^{(0)}$, the subdiagonal (or superdiagonal) to reconstruct $a_1(r)$ and so forth. The matrix $B_{p,q}$ and the elements $b_n(r)$ are related in a similar manner.

Theorem 3. If $\Omega\subset R^2$ is a bounded circular domain, then there exists at most one solution to the inverse problem (4.2). For exact measurements there exists a solution to the linearised inverse problem about the centre f^*.

Proof. We first consider uniqueness of solution. The preceding part of this section shows that it is only necessary to show uniqueness of solution for (4.6). Consider (4.6) to have a solution in $L^2(0,1)$, that is $a_n(r)$, $b_n(r)\in L^2(0,1)$, then the functions $\{r^{n+2q+1}\}=\{r^{n+1}, r^{n+3}, r^{n+5}, \ldots\}$ are complete in $L^2(0,1)$. The Muntz closure theorem (see [32, p 267]) shows the solutions to (4.6) then must be unique. As $L^\infty(0,1)\subset L^2(0,1)$, it follows that the solution in $L^\infty(0,1)$ is also unique.

The direct proof of existence of solutions to (4.6) for a linearisation about any $f^0\in F(\Omega)$ seems quite difficult; a necessary and sufficient existential condition for a solution a_n in $L^2(0,1)$ in this case is

$$\sum_{q=0}^{\infty}|c_{2q,0}A_{n,0}+c_{2q,1}A_{n+2,2}+\ldots c_{2q,2q}A_{n+2q,2q}|^2<\infty \tag{4.7}$$

where the coefficients $c_{2q,l}$ denote the coefficient of x^l in the power expansion of the $2q$th Legendre polynomial of argument x. A similar inequality must hold for the odd solution b_n when the set $\{A_{n,l}\}$ are replaced by the $\{B_{n,l}\}$ in (4.7).

However, when the measurements are exact we have existence to the non-linear inverse problem as discussed after equation (2.11). Because of the linearisation result of theorem 2, this will imply that there exists a solution to the linearised inverse problem in the event of linearisation about f^*.

5. Numerical solution of a radially symmetric inverse problem

We have developed in §4 a closed form expression for the Fréchet differential when $f=f^0$, namely (4.5). This can be utilised when solving the non-linear problem (2.1) when the *modified* form of the Newton–Kantorovich method is used. In this section we shall apply this method to obtain some numerical results from the reconstruction, of several radially symmetric $f^*(r)$, from boundary measurements on a circle of unity radius. We chose to reconstruct discontinuous f—noting we have proved Fréchet differentiability for $f \in L^\infty(\Omega)$ and positive.

The modified Newton–Kantorovich scheme we use to solve (2.11) is

$$Q'(f^0)s^{(k)} = -Q(f^{(k)}) \qquad f^{(k+1)} = P(f^{(k)} + s^{(k)}) \tag{5.1}$$

given some initial constant and positive estimate f^0. P is as defined in equation (2.8). We see the Fréchet derivative is left fixed as at the first iteration and is *not* updated (compare with (2.12) and (2.8)). Thus we can use the closed form Fréchet differential (4.6) in our scheme, thereby simplifying the computational complexity considerably. We stress we are not advocating this as an approach to be taken in general, but here it enables us to illustrate the computational properties of the Newton–Kantorovich scheme with simple calculations. Our numerical experiments with this method show that, if a good approximation f^0 is known, this procedure greatly simplifies the calculations.

Other authors [34–36] have considered inverse problems involving reconstruction of one-dimensional f. However the methods they use are not as powerful as ours in that either they will not handle discontinuities in f, or the methods cannot be generalised to n-dimensional f.

As the radially symmetric f^* is clearly even in θ, only the even moment equations in (4.6) are needed, where now the a_n and $A_{p,q}$ have an iteration number k appended as a superscript. It follows that on the kth iteration from (4.6) equation (5.1) becomes

$$\int_0^1 r^{2q-1} a_0^{(k)}(r)\, \mathrm{d}r = (f^0)^2 A_{q,q}^{(k)} \qquad 0 \leqslant q \leqslant N. \tag{5.2}$$

In order to solve this linear moment problem it is necessary to approximate the $a_0^{(k)}(r)$ by piecewise constant functions. This is of no numerical disadvantage, as splines of degree zero are the appropriate polynomials to use for the approximation of the discontinuous function f^*. We choose for the f^* to be reconstructed the step function

$$f^*(r) = \begin{cases} 1+a & 0 \leqslant r \leqslant \frac{1}{2} \\ 1 & \frac{1}{2} < r \leqslant 1 \end{cases} \tag{5.3}$$

for various values of the constant a. Table 1 summarises our numerical results when eight uniform intervals on $[0, 1]$ were used for the piecewise constant basis; that is $N=8$. All numerical computations were performed on a PRIME P750 digital computer in single precision. With this precision the machine epsilon, denoted by ε and which is defined as the smallest positive number such that $1+\varepsilon > 1$, is approximately 10^{-7}. All integrals were evaluated with an adaptive Simpson's rule to a relative accuracy of 10^{-6}.

In all cases tested the condition number of the linear algebraic system of equations to be solved was of the order 10^5. In figure 1 we plot the normalised ordered singular values of the matrix resulting from (5.2) when $N=8$. The singular values have been

Table 1. Results of numerical computation with the modified Newton–Kantorovich method showing the accuracy achieved against a and number of iterations.

a	Number of iterations K	$\|f^* - f^{(K)}\|_\infty$
0.1	1	0.010
0.5	8	0.001
1	9	0.031
−0.25	5	0.008

normalised so that the largest one is 1. This figure shows that the singular values are exponentially decreasing, asymptotically. Any practical problem with inexact data, that is with noise present, must therefore use regularisation in order to produce acceptable solutions. This could be incorporated with the Tikhonov selection method of §3 or with the Tikhonov–Miller [23] regularisation method. Murai and Kagawa [13] have in effect utilised this latter method, illustrating that regularisation techniques can be applied to produce results in the presence of noise for this problem.

The order of convergence of our method was linear; as expected for the modified Newton–Kantorovich method. Convergence was monotone for all positive values of a tested, as shown in table 2 for $a = 0.5$. For $a < 0$ the convergence, though remaining linear, changed from monotone to an oscillatory nature. In fact convergence was difficult to achieve for negative a, and the method failed to converge for all $a < -0.3$, illustrating that the problem was too non-linear for the initial linear approximation to be satisfactory for these values of a. We started off with an initial approximation $f^{(0)} = 1$ in all cases. We stress again that, using a full Newton–Kantorovich implementation, where the Fréchet derivative is updated, convergence for these more difficult cases would be expected.

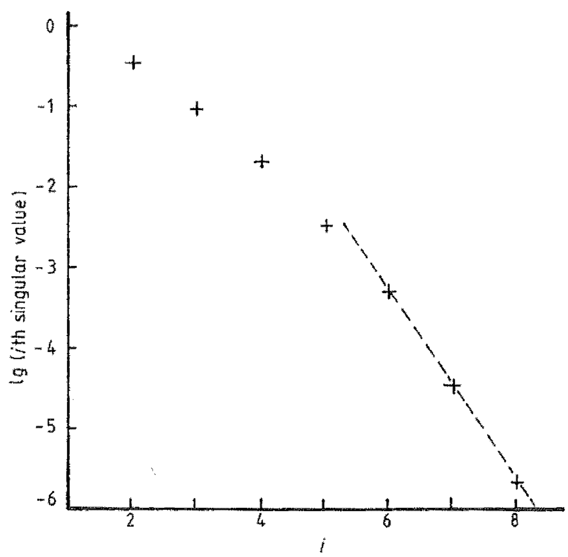

Figure 1. The distribution of lg (ith singular value) against i.

Table 2. Results of numerical computation showing the linear convergence of the method for $a=0.5$, $N=8$.

Iteration number	$\dfrac{\|f^*-f^{(k)}\|_\infty}{\|f^*-f^{(k-1)}\|_\infty}$
1	–
2	0.51
3	0.50
4	0.50
5	0.52
6	0.50
7	0.52

For $a=0.1$ we illustrate in figure 2 the solution obtained after one iteration, i.e. just the solution of the linearised problem as given in (4.2). This figure illustrates how, for small perturbations, the linearised model can give remarkably good results.

Acknowledgment

T J Connolly acknowledges the receipt of a NZ UCG Postgraduate Scholarship.

Appendix

Use has been made of the following generalisation of the Green theorems (see [37, p 127]). The first theorem is as follows.

If Ω is regular bounded region, and $u_1, f \in C^1(\Omega)$, $u_2 \in C^2(\Omega)$ then

$$\int_\Omega u_1 \nabla \cdot (f \nabla u_2)\, \mathrm{d}x = -\int_\Omega f \nabla u_1 \cdot \nabla u_2\, \mathrm{d}x + \int_{\partial\Omega} f u_1 \frac{\partial u_2}{\partial v}\, \mathrm{d}S. \tag{A1}$$

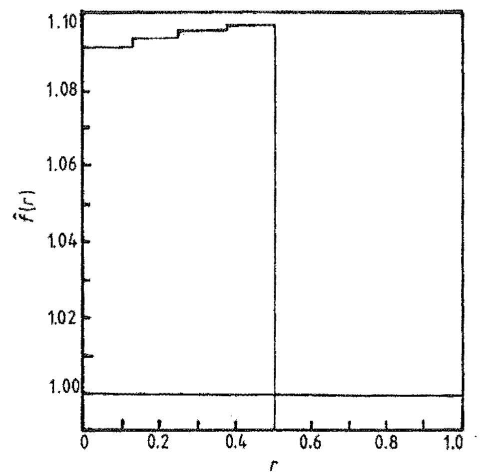

Figure 2. Solution $\hat{f}$ from the linearised problem, when $a=0.1$ in (5.1).

When Ω is a regular its boundary $\partial\Omega$ is a piecewise smooth orientable surface. A surface $\partial\Omega$ is smooth if it has a unique normal whose direction depends continuously on points of $\partial\,\Omega$. The second theorem:

$$\int_{\Omega} [u_1\nabla\cdot(f\nabla u_2)-u_2\nabla\cdot(f\nabla u_1)]\,\mathrm{d}x=\int_{\partial\Omega} f\left(u_1\frac{\partial u_2}{\partial v}-u_2\frac{\partial u_1}{\partial v}\right)\mathrm{d}S. \qquad \text{(A2)}$$

where now $u_1\in C^2(\Omega)$ also.

References

[1] Bates R H T, McKinnon G C and Seagar A D 1980 A limitation on systems for imaging electrical conductivity distributions *IEEE Trans. Biomed. Eng.* **19** 418–20

[2] Price L R 1979 Electrical impedance computed tomography (ict): a new c.t. imaging technique *IEEE Trans. Nucl. Sci.* **26** 2736–9.

[3] Barber D C and Brown B H 1984 Applied potential tomography *J. Phys. E: Sci. Instrum.* **17** 723–32

[4] Dines K A and Lyttle R J 1981 Analysis of electrical conductivity imaging *Geophysics* **46** 1025–36

[5] Richter G R 1981 An inverse problem for the steady state diffusion equation *SIAM J. Appl. Math.* **41** 210–21

[6] Chavent G 1973 Identification of distributed parameters *Proc. Third IFAC Symp.* ed P Eykhoff (Amsterdam: North-Holland)

[7] Ramm A G 1987 Necessary and sufficient conditions for a function $A(\theta', \theta, k)$ to be a scattering amplitude corresponding to a reflecting obstacle *Inverse Problems* **3** L53–7

[8] Kohn R V and Vogelius M 1984 Determining conductivity by boundary measurements *Commun. Pure Appl. Math.* **37** 289–98

[9] Kohn R V and Vogelius M 1984 Identification of an unknown conductivity by measurements at the boundary *SIAM Proc.* vol 19, ed D W McLaughlin pp 113–23

[10] Kohn R V and Vogelius M 1985 Determining conductivity by boundary measurements II, interior results *Commun. Pure Appl. Math.* **38** 643–67

[11] Sylvester J and Uhlmann G 1986 A uniqueness theorem for an inverse boundary value problem in electrical prospection *Commun. Pure Appl. Math.* **39** 91–112

[12] Sylvester J and Uhlmann G 1987 A global uniqueness theorem for an inverse boundary value problem *Ann. Math.* **125** 153–69

[13] Murai T and Kagawa Y 1985 Electrical impedance computed tomography based on a finite element model *IEEE Trans. Biomed. Eng.* **43** 788–803

[14] Yorkey T J and Webster J G 1987 A comparison of impedance tomographic reconstruction algorithms *Clin. Phys. Physiol. Meas.* **8** 55–62

[15] Breckon W R and Pidcock M K 1987 Mathematical aspects of the impedance imaging *Clin. Phys. Physiol. Meas.* **8** 77–84

[16] Connolly T J, Wall D J N and Bates R H T 1985 Inverse problems and the Newton-Kantorovich method *Proc. Int. Soc. Optical Eng.* vol 558, ed R H T Bates and A J Devaney pp 30–4

[17] Chen Y M and Lui J Q 1982 A numerical algorithm for solving inverse problems of two-dimensional wave equations *J. Comp. Phys.* **50** 193–208

[18] Lui J Q and Chen Y M 1984 An iterative algorithm for solving inverse problems of two-dimensional diffusion equations *SIAM J. Sci. Stat. Comp.* **5** 255–69

[19] Roger A 1981 Newton-Kantorovich algorithm applied to an electromagnetic inverse problem *IEEE Trans. Antennas Propag.* **29** 232–8

[20] Volevitch L A and Paneyakh B P 1965 Certain spaces of generalised functions and embedding theorems *Russ. Math. Survey* **20** 1–73

[21] Gilbarg D and Trudinger N S 1983 *Elliptic Partial Differential Equations of Second Order* (Berlin: Springer)

[22] Tréves F 1975 *Basic Linear Partial Differential Equations* (New York: Academic)

[23] Tikhonov A N and Arsenin V Y 1977 *Solutions of Ill-posed Problems* (Washington, DC: Winston)

[24] Adams R A 1975 *Sobolev Spaces* (New York: Academic)

[25] Colton D 1984 The inverse scattering problem for time-harmonic acoustic waves *SIAM Rev.* **26** 323–50

[26] Colton D and Kress R 1983 *Integral Equation Methods in Scattering Theory* (New York: Wiley)

[27] Kravaris C and Seinfeld J H 1985 Identification of parameter systems by regularisation *SIAM J. Control Opt.* **23** 217–41

[28] Bertero M, De Mol C and Viano G A 1979 The stability of inverse problems *Inverse Scattering Problems in Optics* ed H P Baltes (Berlin: Springer) pp 116–24

[29] Dennis J E and Schnabel R B 1983 *Numerical Methods for Unconstrained Optimisation and Nonlinear Equations* (Englewood Cliffs, NJ: Prentice-Hall)

[30] Fedotowsky A, Boivin G and Tremblay R 1971 Inversion of microwave scattering patterns *Can. J. Phys* **49** 3082–94

[31] Cohen J K and Bleistein N 1977 An inverse method for determining small variations in propagation speed *SIAM J. Appl. Math.* **32** 784–99

[32] Calderon A P 1980 On an inverse boundary value problem *Seminar on Numerical Analysis and its Applications to Continuum Mechanics* (Rio de Janeiro: Soc. Brasileira de Matematica) pp 65–73

[33] Davis P 1963 *Interpolation and Approximation* (New York: Blaisdell)

[34] Coen S and Yu M W-H 1981 The inverse problem of the direct current conductivity profile of a layered earth *Geophysics* **46** 1702–13

[35] Langer R E 1933 An inverse problem in differential equations *Bull. Am. Math. Soc.* **39** 814–20

[36] Langer R E 1936 On the determination of earth conductivity from observed surface potentials *Bull. Am. Math. Soc.* **10** 747–54

[37] Williams W E 1980 *Partial Differential Equations* (Oxford: Clarendon)